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Chemistry and French Philosophy of Science. A Comparison of Historical and Contemporary Views

Abstract

Philosophers of science have shown over the past several years a growing interest in chemistry. Chemistry has always held an important place in French philosophy of science. By confronting our respective experiences as philosopher and chemist, we bring out the specificity of the French tradition. The insight provided thereby will allow us to examine afresh some philosophical problems raised by contemporary science: changing conceptions of matter, laboratory practice as opposed to mathematical representation as well as the impact of computer modeling and atomic microscopy on our knowledge of the behavior of matter.

1. Introduction

Since the 1990s there has been a significant attempt to promote a reflection especially devoted to chemistry. One may point to the founding of an international society and two journals in this area: the International Society for the Philosophy of Chemistry (1997), *Hyle: International Journal for Philosophy of Chemistry* (1995), *Foundations of Chemistry* (1999). This movement is a reaction against the neglect of chemistry in mainstream philosophy of science. Current interest in this science may be viewed as a late consequence of the critique of logical empiricism, which has led to pay greater attention to concrete, practical or technical aspects of science.

Now chemistry has held an important place in French philosophy of science. When philosophy of science was just beginning to emerge in the 18th century, such prominent thinkers as Jean-Jacques Rousseau and Denis Diderot wrote some substantial texts on chemistry. Later, in 1835, Auguste Comte devoted five lessons of his *Cours de philosophie positive* to what he called "Chemical philosophy".[1] In the aftermath several French thinkers paid attention to this science: Pierre Duhem, Émile Meyerson, Gaston Bachelard, Hélène Metzger, and more recently François Dagognet, Bernadette Bensaude-Vincent, Isabelle Stengers. We shall focus on the former three, because they established contemporary philosophy of chemistry. In-

1 Auguste Comte, *Cours de philosophie positive* (1839–1842), 2 vols., Paris: Hermann 1998. Abridged translation H. Martineau, *The Positive Philosophy of Auguste Comte*, 2 vols., Cambridge: Cambridge University Press 2009.

H. Andersen et al. (eds.), *New Challenges to Philosophy of Science*, The Philosophy of Science in a European Perspective 4,
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deed, Duhem, Meyerson and Bachelard offered significant studies of the chemist's approach. And, by examining their conceptions, we can bring out some characteristic features of the French tradition.

We have chosen to take up our topic by drawing on our respective areas of competence as philosopher and chemist. Let us explain this choice.

1.1 A philosopher's motives

As a philosopher I am sensitive to the call for a broader perspective with respect to the sciences. The philosopher can no longer remain content with a formal analysis of science nor restrict herself to those fields that submit easily to such a task. She should henceforth take into account the diverse results of science studies (historical, sociological, philosophical, anthropological, etc.) as well as the numerous methods employed in the sciences.

In this respect chemistry raises questions that are of primary interest to the philosopher: the relations between the organic and the inorganic, the nature of the basic stuff of the universe, the effect of drugs on us, the promise or the fright raised by nanotechnology.

1.2 A scientist's motives

As a chemist I expect from the philosopher a better understanding of what distinguishes chemistry from the other natural sciences, those bordering on its domain: physics, biology, the earth sciences, etc. It is important to grasp the philosophy that underlies this science – a question that involves chemistry's relation to society. This quest for meaning is not without practical import, as it may provide clues to two problems:

(1) Why is chemistry so often relegated to the margins of the so-called exact sciences? Why is it invariably given a bad reputation – both by the lay public and by scientists – associating it with the "dark ages" of alchemy and magic? In particular, why is it that, as society becomes more critical of techno-science, chemistry is designated as the culprit, retaining from a bygone era a quasi-malefic image? This is a reputation which it cannot get rid of in spite of its success in areas such as the medical or environmental sciences, for example. And this holds regardless of the ever greater recourse to the methods of physics, which are well-established on the theoretical level. In other words, can we make clear the connections between chemistry – its ontology, its epistemology – and the other sciences as well as its connections with society?

(2) What are the consequences of recent discoveries with which physicists and computer scientists have provided the chemist? I am referring to certain innovations in microscopy, on the one hand, and to supercomputers, on the other. How are these going to modify the representations that first the chemist and then the lay person are coming to have of the atomic and molecular world? This is a fundamen-

tal issue, which is bound to have, in my opinion, an effect on the creativity of the chemist, our conception of matter and the way chemistry is taught.

In response to these questions, can we find clues in the philosophical reflections on chemistry for advancing our comprehension of current chemistry – a science which claims to handle atoms and molecules at the nanoscopic level?

2. Rousseau and Diderot: Chemistry as an epistemological model

Jean-Jacques Rousseau (1712–1778), following Georg Ernst Stahl, conceived of chemistry by analogy with mechanics and according to the general principles of attraction and repulsion among bodies as evidenced in his *Chemical Institutions* of 1747. At the same time, this science was clearly set apart, because chemistry "makes it possible to reach a true knowledge of nature, that is the bodies that compose it".[2] Chemistry was then as much a science that transforms bodies as one that separates them, since each stage of separation can be conceived as a transformation. Analysis, understood as the transformation of bodies, is carried out by a series of manipulations, that is literally manual operations, before becoming a mental procedure. Rousseau dwelled on the concepts of "mixt" and "aggregate"[3] which he distinguished precisely: in mixed bodies the original properties of a constituent are no longer recognizable. "Mixion" consists then in an alteration, whereas "aggregation" is a composition obeying a strict logic of immanence. This contrast became a paradigm for Rousseau's political concepts of association and body.[4] To sum up, as stated by Bruno Bernardi, Rousseau's approach is "a regional philosophy of chemistry"[5], which sets chemistry apart from the other natural sciences.

2 Jean-Jacques Rousseau, *Les institutions chimiques* (1747), Paris: Champion 2010, I, ch. 1, p. 10, our translation. Cf. Bruno Bernardi, "Pourquoi la chimie? Le cas Rousseau", in: *Revue Dix-huitième siècle* 42, 2010, pp. 433-443.

3 Following Louis-Bernard Guyton de Morveau, who wrote: "Aggregation is merely the union of several parts of a similar body without decomposition, and which are called in consequence integrated parts […]. Affinity, in contrast, makes up a new body", our translation. This passage from the *Encyclopédie* is quoted in Bernardi, *La fabrique des concepts*, Paris: Champion 2006, p. 158.

4 Rousseau: "The life of both bodies is the self common to the whole, the reciprocal sensibility and internal correspondence of all the parts. Where this communication ceases, where the formal unity disappears, and the contiguous parts belong to one another only by juxtaposition, the man is dead, or the State is dissolved", *Discours sur l'économie politique*, in: *Oeuvres complètes*, vol. 3, Paris: Gallimard 1964, p. 245. English translation, Constitution Society. Cf. Roger D. Masters and Christopher Kelly (Eds.), *The Collected Works of Rousseau*, vol. 3, Hanover, NH: University Press of New England 1993. See also Luc Vincenti, *Jean-Jacques Rousseau: l'individu et la République*, Paris: Kimé 2001, ch. 5, p. 146.

5 Bernardi, "Pourquoi la chimie?".

Denis Diderot (1713–1784) can also be considered as one of the first philosophers of chemistry. As emphasized by François Pépin[6], he added to his transcription of Guillaume-François Rouelle's lectures[7] a lengthy introduction, in which he situated chemistry – namely its scientificity and philosophical dignity – in historical perspective. Diderot viewed chemistry as a science distinguished not so much by its subject matter but rather its methods; these are formally very different from those of the mechanist. He sought out its specificities, its particular forms of activity – above all laboratory practice, which Diderot contrasts with the activity of mechanics. The latter he classed among the a priori speculations pursued in logico-deductive demonstrations. The methods of chemistry are to be understood in the light of its relations to nature, whose secrets it seeks to reveal by transforming it. These particularities are illuminating:

> You may devote yourself as much as you like to geometry and metaphysics, but I, who am a physicist and a chemist, I study bodies in nature and not in my mind, I see them existing, varied, bearing properties and actions, and moving about in the universe as in the laboratory, where if a spark goes off near three molecules comprising saltpeter, coal and sulfur an explosion will necessarily ensue.[8]

Rousseau and Diderot provide us with examples of a genuine endeavour to understand chemistry not only in terms of its usual objects of study but also its special operations and practices. What we have here is undoubtedly the elaboration of a philosophy of chemistry, a discourse on an area of scientific activity that takes into account its particularities. One notes the distinctive status that chemistry held in the minds of French philosophers of the 18th century. This science likewise played an important role in Kant, who made use of arguments similar to those of Rousseau and Diderot. He conceived of experimental chemistry as more an art than a science and moreover as an analogy for his transcendental idealism:

> So long therefore, as there is still for chemical actions of matter on one another no concept to be discovered that can be constructed, that is, no law of the approach or withdrawal of the parts of matter can be specified according to which, perhaps in proportion to their density

6 François Pépin, "Diderot philosophe de la chimie: des Lumières à la science contemporaine", in: Jean-Pierre Llored (Ed.), *La chimie, cette inconnue?* Paris: Hermann, in press, our translation.

7 Guillaume-François Rouelle (1703–1770) is one of the major French chemists of the 18th century. Many renown members of the French intellectual community, including Lavoisier, attended his lectures on chemistry, which he held in his laboratory. He was associate member of the French Academy of Science. Diderot followed his courses for three years.

8 Denis Diderot, *Principes philosophiques sur la matière et le mouvement* (1770), in: *Oeuvres philosophiques*. Paris: Garnier 1964, p. 395, our translation. See Jean Starobinski, *Action and Reaction*. New York: Zone Books 2003, ch. 2. and Pépin "Diderot: la chimie comme modèle d'une philosophie expérimentale", in: *Revue du Dix-huitième siècle* 42, 2010, pp. 445-472.

or the like, their motions and all the consequences thereof can be made intuitive and presented a priori in space (a demand that will only with great difficulty ever be fulfilled), then chemistry can be nothing more than a systematic art or experimental doctrine, but never a proper science.[9]

3. Duhem: Physical chemistry, axiomatics and the Vienna Circle

Let us now turn to the situation at the beginning of the 20th century. Pierre Duhem (1861–1916), who offered an influential conception in philosophy of science, devoted particular attention to chemistry. In 1902 he published *Mixture and Chemical Combination*, in which he explored the historical development and the philosophical implications of this field.[10] Several other of his works touch on chemistry. This is not surprising as the research program in which Duhem was involved consisted in closing the gap between physics and chemistry, in order to develop a general thermodynamics or energetics, which was supposed to include chemical phenomena. One needs only to read Duhem's major work *The Aim and Structure of Physical Theory* in order to recognize that chemistry is not in the least forgotten.[11] It receives no less attention than electricity, magnetism or optics. Chemistry is mentioned at decisive moments in Duhem's argumentation: the concept of natural classification, the principle of simplicity and the holist thesis.[12]

Of course, Duhem's philosophy of chemistry arose in a particular context. He promoted the application of thermodynamics and in particular the concept of thermodynamic potential in the wake of Helmholtz and Gibbs. Yet Duhem remained hostile to atomism. Indeed, at the time, the multiplication of hypotheses and disagreements between theory and experiment raised much perplexity from the scientific community. To be sure, Duhem's chemistry is that of a physicist. He relied mainly on the tools of thermodynamics. His presentation was modeled on physics and was highly mathematical in style. What we have here, however, is not an attempt at reduction: Duhem provided an example of a unification that maintains the autonomy of the fundamental branches of science. It is important to note that Duhem's axiomatics left room for applied science. As Louis de Broglie remarked in the foreword to the English translation of *The Aim and Structure*: "It

9 Immanuel Kant, *Metaphysical Foundations of Natural Science*, translation M. Friedman, Cambridge: Cambridge University Press 2004, p. 7. See Mai Lequan, *La chimie selon Kant*. Paris: Presses universitaires de France 2000.

10 Pierre Duhem, *Le mixte et la combinaison chimique*. Paris: Fayard 1985. English translation P. Needham, *Mixture and Chemical Combination*. Dordrecht: Kluwer 2002. Cf. Robert Deltete and Anastasios Brenner, "Essay Review of Pierre Duhem's *Mixture*", in: *Foundations of Chemistry* 6, 2004, pp. 203-232.

11 Duhem, *La théorie physique, son objet et sa structure* (1906), Paris: Vrin 1981. English translation P.P. Wiener, *The Aim and Structure of Physical Theory*. Princeton: Princeton University Press 1991.

12 *Ibid*., pp. 25, 127, 214.

is fair to insist on the fact that Duhem, though he was constantly preoccupied with the establishment of an impeccable axiomatic system in the theories he developed, never lost sight of the problems of applications. Notably in the domain of physical chemistry."[13]

The logical positivists or empiricists retained only axiomatics, leaving aside a large portion of Duhem's work. They devoted their attention to those fields to which logical analysis applies best: mathematics and selected parts of physics. The Vienna Circle's manifesto outlined a program which covers many "fields of problems": arithmetic, physics, geometry, biology, psychology and the social sciences (including history and political economy).[14] Chemistry is altogether missing. Although this science is obviously considered rigorous, it does not lend itself easily to an axiomatic treatment. The subsequent development of logical positivism in the *Encyclopedia of Unified Science* gives no reason to change this conclusion; the nineteen volumes of this series, founded by Otto Neurath, which appeared between 1938 and 1970, deal with a large number of sciences, but one does not find anything on chemistry.[15] That there was no chemist among the twenty or so members of the Vienna Circle does not furnish an explanation. Reading over the writings of the logical positivists, one also finds few references to chemistry. Let us quote one passage, however, if only to show that there was no intention of excluding this field from their "scientific worldview". Otto Neurath in the following passage called on chemistry to mark a difference between a genuine scientific inquiry and a mere logical study:

> If we investigate whether the directions of a chemist are in logical agreement, we are not yet doing work in chemistry. In order to be able to do work in chemistry, we must state certain correlations between certain chemical processes and certain temperatures and the like.[16]

Here as elsewhere Neurath criticized his fellow positivists for not paying heed to practice. But let us note especially the slight space allotted to this science. It is surprising that empiricists were not more attentive to the important experimental work accomplished by chemists, as regards both their findings and the concrete procedures they elaborated. It is furthermore strange that self-proclaimed materialists were not more interested in the problem of matter with which chemistry is inevitably involved.

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13 *Ibid*., p. VI.

14 Hans Hahn, Rudolph Carnap and Otto Neurath, "The Scientific Conception of the World: The Vienna Circle", in: Otto Neurath, *Empiricism and Sociology*. Dordrecht: Reidel 1973, pp. 299-318.

15 Neurath provides a presentation of the project in "Unified Science and its Encyclopedia", in: *Philosophical Papers*. Dordrecht: Reidel 1983. Cf. Friedrich Stadler, *The Vienna Circle: Studies in the Origins, Development and Influence of Logical Empiricism*. Springer: Vienna 2001.

16 Neurath, "Sociology in the Framework of Physicalism", in: *Philosophical Papers*, p. 80.

4. Meyerson: The critique of positivism and the defense of atomism

The importance given by Duhem to chemistry would not have exerted an influence, if several major thinkers had not taken up the issues he raised. It is undoubtedly on account of the contributions of Meyerson and Bachelard that chemistry came to acquire its particular place in contemporary French philosophy of science. Émile Meyerson (1859–1933) was trained as a chemist. He was instrumental in spreading the methods and philosophical discussions he had acquired during his studies in Germany. Although Duhem's senior by a few years, he entered the philosophical debate later, his first book *Identity and Reality* being published in 1908.[17] One is not surprised then to see him go to pains to define his position in contrast to Duhem. He vigorously defended atomism as reassessed in the light of recent discoveries. He rejected the positivism of Auguste Comte and Ernst Mach as well as its reformulation by Duhem, and he asserted his own realism. Meyerson offered a different reading of history:

> Neither Galileo nor Descartes are atomists in the strict sense of the term, and amongst later physicists, many, even those who assert that they adhere to this doctrine, formulate its principles in a very different way, often with inexactness, and, in practice, frequently straying from it. Yet it is certain that one can unite all the conceptions under the term *mechanical* [*conceptions mecanistes*] and that their common characteristics are of considerable importance. On the whole, it does not seem too bold to affirm that the mechanical hypotheses had their birth with science and have formed one body with it during all the epochs in which it has really advanced.[18]

Rather than "mechanicist conceptions" some historians today prefer to speak of "kinetic corpuscularianism".[19]

Meyerson did not follow Duhem and Poincaré in conceiving scientific laws as freely chosen postulates. Rather laws are to be understood as the outcome of a struggle opposing the mind's tendency toward identity and the resistance of matter. As Meyerson wrote: "The activity of the mind does not appear to be completely arbitrary, but rather to be guided, on the one hand, by the identification of diversity and, on the other, by the observation of the behavior of concrete reality [*du réel concret*]."[20] Such descriptions are undoubtedly inspired by the practice of the chemist. And Meyerson compared, on more than one occasion, the activity of the scientist to the act of drawing a fiber from the magma of reality. To be sure this

17 Émile Meyerson, *Identité et réalité*. Paris: Vrin 1951. English trans. K. Loewenberg, *Identity and Reality*. London: G. Allan & Unwin 1930.

18 *Ibid.*, p. 88.

19 For example H. Floris Cohen, *How Modern Science Came into the World*. Amsterdam: Amsterdam University Press 2010, p. 221.

20 Meyerson, *Du cheminement de la pensée* (1931), 3 vols., Paris: Alcan, p. 613, our translation.

metaphor is borrowed from the biologist Arthur Balfour.[21] But it applies relevantly to all sciences dealing with complexity.

Meyerson represented the beginning of a shift away from positivism. This was continued by Bachelard, Koyré and their disciples. Positivism was receding in France precisely when positivism was gaining strength in Austria. Meyerson wrote, after becoming acquainted with the doctrine of the Vienna Circle toward the end of his life:

> I deem it useful to summarize here these conceptions as a whole (which appear to enjoy at present a certain success in German-speaking lands) precisely because, on a number of essential points, they go entirely against the views that I have put forth in my earlier writings and that represent the core of this book.[22].

5. Bachelard: Chemistry and applied materialism

It is well known that Gaston Bachelard (1884–1962) distinguished himself more and more clearly as the years went by from Meyerson. His criticism was directed as much at the interpretation of scientific results as their consequences with regard to scientific rationality. This does not mean that Bachelard returned to earlier conceptions; he subscribed to Meyerson's criticism of idealism and positivism as well as his defense of atomism and realism. But he went on to set himself apart from his predecessor and reformulated these positions.

Let us recall a passage of *The Rationalist Activity of Contemporary Physics*, which aims to bring out the consequences of the "new theory of quanta".[23] According to Bachelard, Meyerson's realism is as questionable as the positivism he opposed:

> One is ill-prepared to follow the evolution of modern atomistics if one accepts Meyerson's phrase stating that the atom is merely "strictly speaking a portion of space". This is a ready-made phrase [*formule réponse*] […] which treats lightly the huge problem of modern atomistics. It leaves aside too hastily the prudent restrictions of a positivist mind.[24]

And Bachelard went on to formulate his position: "Corpuscles border on invention and discovery, precisely in the realm in which we believe applied rationalism to be active."[25] If Bachelard claimed to be realist, rationalist and even materialist, it should be understood that his is a constructive realism, an applied rationalism and a rational materialism. He sought to open a new perspective thereby. His scientific

21 *Ibid.*, p. 138. Cf. p. 246.

22 *Ibid.*, p. 790, our translation.

23 Gaston Bachelard, *L'activité rationaliste de la physique contemporaine*. Paris: Presses universitaires de France 1951.

24 *Ibid.*, p. 86, our translation. Cf. Meyerson, *Identity and Reality*, ch. 9.

25 Bachelard, *L'activité rationaliste*, p. 87.

realism has nothing to do with common sense realism, and Bachelard went as far as to speak in the same passage of a "relativism of ontology". As is known, W. V. O. Quine will also transform Meyerson's realism, but in a quite different context.[26] The scientist makes ontological engagements, but one should understand in what sense: he does not hesitate to continuously adjust his ontology to scientific progress.

Bachelard was led to elaborate what he called "phenomeno-technics". Instruments, experimental setups or better laboratories make it possible to create new phenomena, which although artificial can be more significant than natural processes. What is at issue here is an experimental realism which puts emphasis on the concrete context whereby proof is produced. Bachelard then formulated a philosophical conception based on his experience as a school teacher in physics and chemistry at the beginning of his professional career, a conception that was at odds with that of logical positivism.

6. Conclusions

We may now reflect on the position of contemporary chemistry on the basis of these historical elements.

6.1 The relation to matter

Following a hardline positivism, the chemist refrains, at least professionally, from the question of what matter is in itself. Her focus is on the formulation of concepts dealing with understanding chemical reactions and analyses, that is the mechanisms of decomposition and recombination of matter. The major issues are "What is the result of the reaction of A on B?" and "Why does this occur?" or conversely "How to obtain C from certain synthons?"[27] They can also be understood in the light of the recent development of Quantitative Structure-Activity Relationship (QSAR).[28]

The very nature of matter or its essence is not on the agenda. The chemist accepts: first, that matter is made up of atoms which bond together to constitute

26 W. V. O. Quine, *From a Logical Point of View*. Cambridge (Mass.): Harvard University Press 1980, p. 45. For an attempt to combine instruments of analytic philosophy of science and historical epistemology, see Ian Hacking, *Historical Ontology*. Cambridge (Mass.): Harvard University Press 2002.

27 "A synthon is defined as a structural unit within a molecule which is related to a possible synthetic operation, the term was coined in 1967 by E. J. Corey", in Wikipedia.

28 "The basic assumption of all molecule-based hypotheses is that similar molecules have similar activities. This principle is also called Structure-Activity Relationship (SAR). The underlying problem is therefore how to define a small difference on a molecular level, since each kind of activity, e.g. reaction ability, biotransformation ability, solubility, target activity, and so on, might depend on another difference", in Wikipedia.

complex molecular systems and solids, and secondly, that the chemical or physical properties of matter are dependent on the nature of the atoms involved, their spatial arrangements and their motions. She restricts her "deep" exploration of matter to the atoms or more precisely to the electrons of their outermost shells, the so-called valency electrons which are responsible for chemical reactivity.[29]

Bringing together the major issues and paradigms mentioned above with regard to "chemical" matter makes it possible to reformulate the problem that concerns daily the contemporary chemist, that is "What are the relations between composition, structure and the reactivity of atomic constructions?" This question, of a very general nature and common to all forms of chemistry, whether organic, inorganic or hybrid, arises in particular in the case of supra-molecular structures such as proteins, in which molecular self-organization plays an essential role in regard to their functionality.

6.2 On representations, micro-vision and macro-vision

Although physicists and chemists fully agree with regard to the issues and paradigms mentioned, their methodologies or ways of comprehending matter are fundamentally different. At the molecular level the chemist "prefers" to represent directly atomic and molecular constructions, by likening atoms to balls and chemical bonds to solid lines. She builds her reasoning on pictures or figurative representations. The physicist proceeds rather by speculating on reciprocal space, which is associated with energy, and she schematizes matter and its properties with the help of abstract representations directly related to mathematical descriptions.

The origin and import of these differences is essential, because recourse to figurative representations limits the scope of thought to the space defined by the picture which is used. The chemist consequently tends to represent atomic reality in virtue of the paradigm mentioned above by restricting herself to the molecular level. This apprehension of reality may explain why she is suspicious of or even hostile to the complete mathematization of chemical reactions, which, according to her, cannot account for all complexities and subtleties inherent in matter. This characteristic inability of physics to account for chemical reality could be explained, according to her, by the fact that the concrete system involves a large number of atoms, which corresponds to a high degree of freedom.

As the chemist moves up to higher scales, those pertaining to the physical continuum, the media that are conceptualized without recourse to atoms (dimensions above the nanometer), she is obliged to change radically her approach, because she has no other choice in this case but to call on oversimplified abstract mathematico-physical descriptions on the one hand or on empirical knowledge that cannot be mathematized on the other. The transition from discontinuity to

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29 Valency electrons are those which are associated with the highest energy orbital and which are directly involved in chemical reactivity. For more details see the Frontier-Orbital Theory.

continuity in physics is not without difficulties. But whatever these may be, the tool that is used remains mathematics.

It is within this gap between the figurative representation of atoms or molecules and the mathematized representation of macroscopic media that the chemist can assert her specificity, her freedom vis-à-vis the injunction of the logico-deductive powers of mathematics. It is in this gap that the chemist expresses her "art". It seems that we return to the antagonisms between the physicists Duhem and Poincaré and the chemist Meyerson.

We could conclude on this issue by stating that the view of the physicist and that of the chemist continue to be at odds as they were in the 18th and 19th centuries, and that the chemist is assigned to this in-between zone, as it were trapped between a science and an art.

6.3 Recent developments

It is important to acknowledge that recent developments in "numerical" chemistry, which make it possible to simulate structures, atomic trajectories, physical properties and even chemical reactivity of larger and larger sets of atoms could change irreversibly the relation between the model and the representation of reality.

Two factors more than any others appear to be operating in this evolution which could result in a profound mutation. On the one hand, the computer is conceived as a black box, which renders all but completely invisible the mathematics and the models with which it works. In other words, it has become a tool, which, in being used, requires no special ability in mathematical physics. It can be assimilated thus with the majority of analytic instruments which are used daily without any need to know their "deep" principles. On the other hand, the results obtained by numerical procedures are often translated into atomistic representations of matter; one can visualize the atoms and molecules in space, their movements, their rearrangements, etc. What we have is "a journey to the center of matter"! It is difficult to sort things out and to avoid being led to think that this representation is an entirely faithful photograph of reality. The virtual aspect of this representation is not necessarily scrutinized with care. This vision of reality mediated by the computer is furthermore enhanced by the simultaneous development of atomic microscopy, the results of which are equally translated into figurative representations.

This relation to matter relies first and foremost on the confidence placed on the instruments, because they are too sophisticated and too complex to be understood by the non-specialist. Secondly, the easy and readily available pictures tend to diminish the hostility that the chemist consistently shows vis-à-vis a strictly "mechanistic" approach to matter.

It is probable that Duhem, had he lived today, would refer to atoms. But what would he think of the uses made of these new technologies and especially the philosophical consequences of their use? The questions raised by Rousseau, Diderot, Duhem and Meyerson are still on the agenda. And Bachelard's objection to the identification of the atom with a portion of space points to the complexities still inherent in our conceptions of matter. After the breakthrough of quantum mechanics at the beginning of the 20th century, it is obvious that the figurative representation of molecular or atomic systems in a "classical" 3D Cartesian space cannot be fully suitable. Yet it remains the most used picture of matter and its use is still very efficient.

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