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Thinking chemistry out of the box of daily life in the laboratory

What is Philosophy of Chemistry and Why is it Important

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Abstract: Chemistry is a science fundamentally characterized by the ability of making its own study objects. Chemistry's unique sign language and representations of structural formulas are highly predictive tools. These aspects, together with the richness of qualitative models, make chemistry highly attractive for philosophical studies. However, philosophy of chemistry is, within the philosophy of science, a still relatively young discipline.

Keywords: Language of chemistry · Philosophy of science · Qualitative thinking · Reductionism

The aim of this column is to give a very brief introduction – in fact, just a two-page teaser – to a topic that has long been vastly unappreciated by both chemists and philosophers. I am not a philosopher myself, just a chemist who developed an interest for the philosophy of science since the time I was a student. I came to believe that the philosophical (and historical) reflection about chemistry as a science and as cultural achievement at large, as well as about the working and meaning of chemical concepts and models, may significantly contribute to a broader understanding of this central science and, hence, incentivize a more considered approach to chemistry teaching of at all levels.

It is only since the late 1980s to early 1990s that chemistry has become the object of systematic philosophical research. The existence of the academic discipline of the philosophy of chemistry is demonstrated by at least two dedicated journals,[1] many monographies,[2] review articles[3] and specialized international meetings. However, its perception by, and significance for, chemists are still relatively modest, at least in my perception. Many universities will not offer a course on the philosophy of chemistry in regular chemistry curricula, not only because of the rarity or unavailability of corresponding lecturers, but also because of the lacking awareness among chemists that philosophical reasoning about chemistry and chemical concepts could be enriching and inspiring. Why have we arrived at this state of affairs and what are specific aspects of chemistry that would be – and indeed are – unique for philosophical scrutiny?

"*La chimie crée son objet. Cette faculté créatrice, semblable à celle de l'art lui-même, la distingue essentiellement des sciences naturelles et historiques. Les dernières ont un objet donné d'avance et indépendant de la volonté et de l'action du savant*." This famous statement by Marcellin Berthelot goes back to 1876[4] and conveys one of the most important and distinctive quintessences of chemistry as a science. Almost 150 years later, the validity of the comparison of chemistry to art and chemistry's unique standing among the sciences, as stated by Berthelot, are as timely as ever. One could therefore intuitively attach to these features of chemistry far-reaching philosophical connotations, meaning that chemistry would have been eminently suited for philosophical studies. However, as Fritz Paneth, a chemist by training, observed in 1931 in his fundamental article about the epistemic status of the concept of element: "*Discussions of the principal concepts of chemistry are few and superficial, in striking contrast to the many and penetrating investigations into the philosophic foundations of physical theories*".[5] In fact, historically, physics and its developments have been for philosophers clearly more "interesting" than chemistry, the latter being perceived as a purely empirical science with unpretentious philosophical implications. This has been later related to the problem of reductionism, a problem that is still being debated today.[6] The advent of quantum mechanics led Paul A.M. Dirac to 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*".[7] In view of a development of a philosophy of chemistry, this has possibly had deleterious consequences, at least temporarily. In fact, it corresponded to say that chemistry is just a part of physics, thus cementing previous views about chemistry as a non-autonomous science. It is important to note that modern chemistry is more and more taking advantage of the methods of quantum chemistry, in particular density functional theory (DFT). Computational chemistry significantly helps in understanding structures and reaction mechanisms and a rapidly increasing share of publications in the areas of *e.g.* synthesis and catalysis is including computational work. This does not mean, however, that the whole of chemistry is amenable to a complete mathematization as it may happen in physics and as originally anticipated by Dirac. What distinguishes chemistry from physics are, most prominently, chemistry's experimental methods, in particular those of synthetic chemistry. A chemist can plan and carry out syntheses, draw conclusions, and produce new fundamental knowledge that may be immediately well ahead of what can be deducted from theoretical considerations based on quantum mechanics. This is also the expression of chemistry's highly developed *qualitative thinking* that continues to pervade it and that is difficult to grasp for a non-chemist. To remain in the context of quantum theory, think for example of the idea of an "empty orbital", as commonly used by chemists when discussing *e.g.* the simple interaction between a borane and an amine. While it can be argued that an "empty orbital" is not an existing, observable physical entity in quantum-mechanical terms, it is an extremely useful concept for chemists.

A further very distinctive feature of chemistry is its *language*. By "language" I mean much more than mere systematic nomenclature of compounds which is actually only a part of it and arguably not necessarily the most significant. The language of chemistry as a mean of communicating about chemical objects relies on representations of molecular structures.[8] It has been very wisely claimed that "*the chemical sign language is actually one of the most powerful predictive theories of science at all!*"[9]

What this strong and somewhat astonishing statement conveys, had been already realised by the great philosopher Ernst Cassirer as early as 1929. Cassirer noted that, "*in general, the scientific value of a [structural] formula is not only that it unites given empirical facts, but that it lures out, so to speak, new facts. It puts forward problems about relations, connections, and formation of order, which precede immediate observation*".[10] The process of "luring out" (German: "hervorlocken") new facts from the drawing of a molecule, be it a known one, natural or unnatural, or one that still needs to be made, consists in making predictions about properties and, mainly, reactivity. Fig. 1 shows, for example, how the formation of pyrazoles from 1,3-diketones and a hydrazine is pictorially "lured out" from an appropriate representation of the structure of the two reacting starting materials. It is taken from an organic chemistry textbook by Victor Grignard, [11] which appeared around the time when Cassirer had his fundamental insight about the predictive reading of structural formulas.

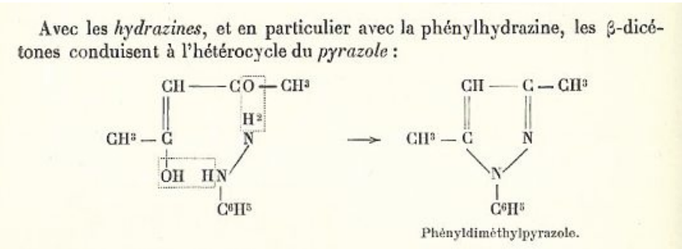

Fig. 1. "Luring out" the formation of pyrazoles from a 1,3-diketone and a hydrazine, as represented in a textbook of Victor Grignard.[11]

This is a fundamental aspect at the heart of *e.g.* retrosynthetic analysis, much in the sense of thought experiments. The prediction of reactivity takes advantage of another essential feature of chemistry, *i.e.* the classification of pure compounds based on their structure and functional group reactivity which is defined according to an operational approach relying on purification procedures. As pointed out by Schummer[9] the "*chemical network, with chemical substances as the nodes and chemical relations as the connections, forms the chemical core of experimental chemistry*". Thus, such a network constitutes the logical structure of what we know about chemical substances.[12]

Whereas the synthesis of essentially any molecule can be planned and potentially realised in the laboratory, the design of its functions, in particular in biological systems, is still very much lagging behind. In fact, in order to find *e.g.* a new drug, one has to go through the cumbersome process of testing many drug candidates. The advent of Artificial Intelligence in chemistry might radically change this situation. However, chemists and machines will have to agree upon a common language. Will this lead to a drastic evolution of the qualitative models of chemistry?[13] Also a philosophically relevant question!

Have fun thinking (about) chemistry!

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[1] Journals: a) *HYLE – International Journal for Philosophy of Chemistry*, http://www.hyle.org/index.html, since 1995; b) *Foundations of Chemistry – Philosophical, Historical, Educational and Interdisciplinary Studies of Chemistry*, https://www.springer.com/journal/10698/, since 1999.

[2] To assist the interested reader, a selection of monographies is given in chronological order of publication: a) P. Janich (Hg.), *Philosophische Perspektiven der Chemie, 1. Erlenmeyer Kolloquium der Philosophie der Chemie*, BI-Wissenschaftsverlag, **1994**; b) P. Janich, N. Psarros (Hg.), *Die Sprache der Chemie, 2. Erlenmeyer Kolloquium zur Philosopihe der Chemie*, Königshausen & Neumann, **1996**; c) P. Janich, N. Psarros (Eds.), *The Autonomy of Chemistry, 3. Erlenmeyer Kolloquium zur Philosophie der Chemie*, Königshausen & Neumann, **1998**; d) N. Psarros, *Die Chemie und ihre Methoden – Eine philosophische Betrachtung*, Wiley, **1999**; e) J. van Brakel, *Philosophy of Chemistry*, Leuven University Press, **2000**; f) J.E. Earley, Sr. (Ed.), *Chemical Explanation – Characteristics, Development, Autonomy, Annals of the New York Academy of Science*, Vol. 988, **2003**; g) D. Baird, E. Scerri, L. McIntyre (Eds.), *Philosophy of Chemistry – Synthesis of a New Discipline, Boston Studies in the Philosophy of Science*, Vol. 242, Springer, **2006**; h) B. Bensaude-Vincent, J. Simon, *Chemistry – The Impure Science*, 2nd Ed., Imperial College Press, **2012**; i) A. I. Woody, R. Findlay Hendry, P. Needham (Eds.), *Handbook of the Philosophy of Science*, Vol. 6, *Philosophy of Chemistry*, Elsevier, **2012**; j) J.-P. Llored (Ed.), *The Philosophy of Chemistry – Practices, Methodologies, and Concepts*, Cambridge Scholars Publishing, **2013**; k) E. Scerri, G. Fisher (Eds.), *Essays in the Philosophy of Chemistry*, Oxford University Press, **2016**; l) B. Bensaude-Vincent, R.-E. Eastes (Eds.), *Philosophie de la chimie*, De Boeck Supérieur, **2020**; m) E. Scerri, E. Ghibaudi (Eds.), *What is a Chemical Element?*, Oxford University Press, **2020**.

[3] For introductory reviews, see: a) J. Schummer, *Endeavour* **2003**, *27*, 37-41, https://doi.org/10.1016/S0160-9327(03)00004-8; b) J. Schummer, *Philosophie der Chemie*, in *Grundriss Wissenschaftsphilosophie*, S. Lohse, T. Reydon (Hg.), Meiner, **2017**, S. 229-251; c) M. Weisberg, P. Needham, R. Hendry, *Philosophy of Chemistry*, in *The Stanford Encyclopedia of Philosophy*, E. N. Zalta, (Ed.), **2019**, https://plato.stanford.edu/archives/spr2019/entries/chemistry/. See also the collection of articles by Roald Hoffmann: J. Kovac, M. Weisberg (Eds.), *Roald Hoffmann on the Philosophy, Art, and Science of Chemistry*, Oxford University Press, **2012**.

[4] *Chemistry creates its object. This creative faculty, similar to that of art itself, essentially distinguishes chemistry from the natural and historical sciences. The latter have an object given in advance and independent of the will and action of the scientist* (my translation). M. Berthelot, *La synthèse chimique*, 2ème Ed., Librairie Germer Baillière, Paris, **1876**, p. 275.

[5] F. A. Paneth, *British Journal for the Philosophy of Science* **1962**, *13*, 1-14 and 144-160. These articles are a posthumous translation of the original published many years before in German: "*In einem auffallenden Gegensatz zu den vielen und eindringenden Untersuchungen über die philosophischen Grundlagen physikalischer Theorien steht die geringe Zahl und Tiefe der Erörterungen über die chemischen Hauptbegriffe.*" See: *Schriften der Königsberger Gelehrten Gesellschaft*, *Naturwissenschaftliche Klasse* **1931**, Band 8, Heft 4, S. 101-125.

[6] See *e.g.*: a) H. Primas, *Chemie in unserer Zeit* **1985**, *19*, 109-119 and 160-166. b) C. Liegener, G. Del Re, *Zeitschrift für allgemeine Wissenschaftstheorie* **1987**, *18*, 165-174.

[7] P. A. M. Dirac, *Proc. Royal Soc. London* **1929**, *A123*, 714-733.

[8] R. Hoffmann, P. Laszlo, *Representation in Chemistry*, *Angew. Chem. Int. Ed. Engl.* **1991**, *30*, 1-16, https://doi.org/10.1002/anie.199100013.

[9] J. Schummer, *The Chemical Core of Chemistry I: A Conceptual Approach*, *HYLE* **1998**, *4*, 129-162.

[10] E. Cassirer, *Philosophie der symbolischen Formen, 3. Teil: Phänomenologie der Erkenntnis*, Gesammelte Werke, Hamburger Ausgabe, Band 13, Meiner, **2002**, S. 509. The quoted English version of Cassirer's statement is taken from ref. [9], p.161. Original in German: "*Die Chemie ist zur "exakten" Wissenschaft nicht nur durch die ständige Verfeinerung ihrer Massmethoden geworden, sondern vor allem auch durch die Verschärfung dieses ihres gedanklichen Instruments, durch den Weg, den sie von der einfachen chemischen Formel bis zur Strukturformel durchmessen hat. Ganz allgemein besteht der wissenschaftliche Wert einer Formel nicht nur darin, dass sie gegebene empirische Tatbestände zusammenfasst, sondern dass sie neue Tatbestände gewissermassen hervorlockt. Sie stellt Probleme von Zusammenhängen, von Verknüpfungen und Reihenbildungen auf, die der unmittelbaren Beobachtung vorauseilen. So wird sie zu einem der hervorragendsten Mittel dessen, was Leibniz die "Logik der Entdeckung", die logica inventionis, genannt hat"*.

[11] V. Grignard, *Précis de Chimie organique*, Masson, Paris, **1937**, p. 468.

[12] For philosophical reflections, see: K. Ruthenberg, J. van Brakel (Eds.), *Stuff – The Nature of Chemical Substances*, Königshausen & Neumann, **2008**.

[13] See, *e.g.*: T. Clark, M. G. Hicks, *Models of Necessity*, *Beilstein J. Org. Chem.* **2020**, *16*, 1649, https://doi.org/10.3762/bjoc.16.137.