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Philosophical Aspects of Mathematical Chemistry

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After lecturing at the *Second Mathematical Chemistry Workshop of the Americas*[1], organised by Guillermo Restrepo and José L. Villaveces in Bogota (Colombia) in July 2010, Joachim Schummer, editor-in-chief of *HYLE--International Journal for Philosophy of Chemistry*[i] (HYLE), discussed with Restrepo the possibility of editing a special issue of HYLE devoted to philosophical and historical aspects of mathematical chemistry and, more general, the relationship between chemistry and mathematics. In the first HYLE issues of each 2012 and 2013, nine papers were published[2] collecting the thoughts, reflexions and investigations by leading scholars in mathematical chemistry and philosophy of chemistry. As a response, Ivan Gutman, editor-in-chief of *MATCH Communications in Mathematical and in Computer Chemistry*[ii] (MATCH), invited Restrepo to write a document for MATCH commenting about the HYLE issues. In the following lines, we summarise our experience editing the two issues and use the opportunity to ponder on some unsolved questions in the philosophy of mathematical chemistry.

Late recognition

At about the second half of the 20th century, mathematical chemistry began to be recognised as a new discipline and currently counts on specialised books and scientific journals, an academy and regular conferences that gather an international community sharing a common language and scientific interests[3,4,5], which are important criteria for discipline formation[6].

As a first question, several authors asked why the recognition of mathematical chemistry as a discipline was delayed, in contrast particularly to the case of mathematical physics. According to Restrepo and Schummer[3], the delay was due to the

[i] One of the two international journals devoted to Philosophy of Chemistry (URL: http://www.hyle.org, open access), the other one being *Foundations of Chemistry*.
[ii] One of the three international journals devoted to Mathematical Chemistry, *Journal of Mathematical Chemistry* and the *Iranian Journal of Mathematical Chemistry* being the other two.

different epistemologies of chemistry and mathematics, which is related to Immanuel Kant's[7] distinction between *a priori* and *a posteriori* knowledge. For Kant, mathematics is based on *a priori* knowledge; it is abstract and developed by reason without reference to experimentation. In contrast, experiments play such a fundamental role in chemistry that knowledge is hardly accepted after supporting experiments have been conducted, i.e. *a posteriori*. The distinction underlies Kant's position on chemistry and mathematics, well known in the mathematical chemistry community: "chemistry can become nothing more than systematic art or experimental doctrine, but never a proper science; for the principles of chemistry are merely empirical and admit of no presentation *a priori* in intuition"[7]. However, it has been shown that the idea of mathematics as a pure *a priori* science is difficult to maintain, for even the roots of several mathematical branches are founded in *a posteriori* knowledge[8] that has later been generalised and abstracted.

Douglas J. Klein[9] gives two further reasons for the delay in the recognition of mathematical chemistry as a discipline: i) the framing of mathematical chemistry as part of physical chemistry and other areas and ii) the little recognition of non-numerical mathematics as constitutive parts of mathematics. He points to a long and rich history of mathematical chemistry in more than 20 areas of chemistry, which coincides with Ugi and co-workers'[10] opinion that the delay of mathematical chemistry is rooted in the view that chemistry would be part of physics. The issue of whether chemistry is reducible to physics has been one of the recent topics in philosophy of chemistry, as noticed by Schummer in a survey of the field[11].

Klein's second reason for the delay refers to the narrow understanding of mathematics in chemistry, which is also evident in other disciplines as noticed by Kemeny[12], who found still in the 1950s the widespread idea that mathematics would only be about numbers and space. In his paper "Mathematics without numbers"[12], Kemeny tried to eradicate that misconception by pointing to many fields of mathematics that do not depend on numbers, e.g., topology, graph, group and order theories, which incidentally figure prominently in today's mathematical chemistry.

The recognition of mathematical chemistry as a discipline followed different paths in the chemical and mathematical communities, which Restrepo and Villaveces discuss for the particular case of discrete mathematical chemistry[13]. They comment on the initial flat rejection in chemical circles, which led to the establishment of the aforementioned journals, books, meetings and other items shaping the field. Regarding mathematics, the authors conclude that there was more acceptance from that community than from chemistry.

Applied mathematics?

Another question discussed in the two HYLE issues refers to the relationship that mathematical chemistry establishes between mathematics and chemistry, namely whether it is a one-sided utilitarian relationship of mathematics to chemistry ("mathematics as a tool") or whether both sciences benefit from it. Kant is often mentioned by mathematical chemists[14],[15],[16] when discussing applications of mathematics to chemistry. The philosopher is blamed for his claim that chemistry is "incapable of the application of mathematics"[7], which, we think, reflects only his early view on the epistemological and conceptual distance between chemistry and mathematics. However, when criticizing Kant, arguing that mathematics can indeed be applied to chemistry as illustrated by many cases, mathematical chemists implicitly assume and reinforce a one-sided utilitarian relationship. In contrast, Kant himself did not look for mathematical tools to be applied to chemistry but instead for mathematical concepts within chemistry, which he could not found at first. Morever, van Brakel[17] has shown that Kant's opinion on the relationship between chemistry and mathematics has to be updated, because he changed his mind in his later years when he found elements of mathematics in chemistry[8]. Unfortunately, his late position is little known in the English-speaking world because of the long delay of the English (and still abridged) translation[17]. Our message, regarding Kant, for the mathematical chemistry community is that the philosopher has to be understood in a broader sense, rather than just blaming him by quoting his statement on missing mathematical applications to chemistry. The discussion could go further by pondering on the meaning of applied science, in general, and applied mathematics, in particular.

Another classical philosophical view on the relationship between mathematics and chemistry frequently cited by mathematical chemists[15,16] as well as historians and philosophers of science[18] is the one by Auguste Marie François Xavier Comte: "Every attempt to refer chemical questions to mathematical doctrines must be considered, now and always, profoundly irrational, as being contrary to the nature of the phenomena"[19], which follows Kant's distinction between *a priori* and *a posteriori* knowledge. As with Kant, mathematical chemists little discuss other thoughts of Comte; for example his claim that "an inorganic body, possessing solidity, form, consistency, specific gravity, elasticity, etc., presents qualities which are within our estimate, and can be treated mathematically; but the case is altered when Chemical action is added to these. Complications and variations then enter into the question which at present baffle mathematical analysis"[19]. The quotation illustrates his limited understanding of mathematics as merely related to numbers as well as his idea that it is the complexity of chemistry that hinders its mathematization. One is tempted to group Comte with those scholars mentioned by Kemeny[12], who see in mathematics only the study of numbers and space. However, mathematics started to explore and develop its manifold non-numerical branches only at the end of the 19th century after Comte; for example, Cantor introduced the fundamental concept of sets as late as 1895[20]. Moreover, authors criticizing Comte's first quote might not realise that he pointed out the importance of mathematical methods for chemistry rather than of specific fields of mathematics, when claiming for instance: "besides that mathematical study is the necessary foundation of all positive science, it has a special use in chemistry in disciplining the mind to a wise severity in the conduct of analysis: and daily observation shows the evil effects of its absence"[19].

Hence, through a very particular reading of Kant and Comte, the relationship between mathematics and chemistry is traditionally viewed one-sidedly, as one being at best applied to the other. That is why it is not surprising to find statements like "chemistry will […] become a branch of applied mathematics", as claimed by Alexander Crum Brown[21] in 1875. No substantial differences appear in more recent claims by mathematical chemists where the recurrent terms to describe the relationship between mathematics and chemistry are "use" and "application"[14,15].

However, other chemists, such as Ugi and co-workers[10], refer to the logic of mathematics rather than to its specific branches, claiming that "little use [in chemistry] has generally been made of the fact that mathematics is formalized logical thought and can be used directly to gain insight into the intrinsic logical structure behind chemical problems". Following this thread of thought, Restrepo and Villaveces[22] suggest that mathematical chemistry entails the use of the mathematical way of thinking in chemistry, i.e. selecting relevant variables when treating chemical questions, symbolizing and relating them through mathematical functions.

Depending on how one sees the relationship between chemistry and mathematics as established by mathematical chemistry, different views are possible on which discipline benefits from that relationship. In his HYLE paper, Haruo Hosoya, who rejects the idea of mathematical chemistry being simply an application of mathematics to chemistry, shows how issues of mathematical chemistry also inspired mathematical work[23]. For instance, his Z-index, originally devised to describe molecular structures, has helped to visualise and develop abstract features of mathematical number theory. Or, group theoretical approaches to the understanding of fullerenes have assisted the mathematical theory of regular polyhedra. Basak[24] and Restrepo and Villaveces[13,22] point to the chemical roots of graph theory in the works of Sylvester. Schummer[25] argues that the mathematical theory of symmetry originated from crystallography. Klein[9] mentions several mathematical spin-offs from chemical issues, e.g. foundational combinatorial theory of enumeration under group-mediated equivalences, Onsager's solution of the 2-dimensional Ising model, Ruch and Schönhofer's symmetry chirality characterizations and Eyring and Polanyi's ideas of "navigation" on complex potential-energy hyper-surfaces deriving mathematics in dynamical systems. Balaban, in his HYLE paper[26], discusses how exploring the mathematics of reaction graphs led him to discover two unknown graphs of the particular family of cages.

Despite many examples of benefits for mathematics, chemistry has certainly benefited most from mathematical chemistry, as shown by Restrepo and Villaveces[13] and Klein[9]. Klein provides a comprehensive list of cases of mathematical chemistry work in areas such as thermodynamics, statistical mechanics, electrochemistry, quantum chemistry, chemical kinetics, spectroscopy, crystallography, solid-state chemistry, polymer statistics, chemical reaction networks, structure generation and enumeration, chemical classification, chemometrics and chemoinformatics, to name but a few[iii]. Restrepo and Villaveces[13] argue that the still modest impact of mathematical chemistry on mathematics is also due to the recent recognition of the discipline. According to Klein[9] the mathematics behind mathematical chemistry can be obscured by the chemical context, "so that even if something is mathematically very fundamental, it may take some time to be so recognized".

Seeking for a definition

Another topic treated in several of the papers published in the two HYLE issues is the definition of mathematical chemistry. As mentioned before, Restrepo and Villaveces[22] define mathematical chemistry as an approach to chemistry that employs the mathematical way of thinking. Klein[9] requires that mathematical chemistry involves novel mathematical ideas and concepts adapted to or developed for the use in chemistry. His definition rejects the mere use or application of mathematics in chemistry, such as statistics for error estimates or any branch of mathematics without understanding its details and limits[9]. In his own words, that definition "distinguishes mathematical chemistry somewhat from simple routine mathematics for chemical problems and even from rather complex mathematics used repeatedly in some standardized manner (perhaps in the form of a 'canned' computer program)"[9].

Schummer[25] suggests that the subject is best defined by its specific methodological approach to develop mathematical theories of chemistry that do without claims about causal structures and without aspiring to develop one unifying theory. The first condition allows drawing a clear distinction from physical chemistry and mathematical physics, the lack of which might be another reason for the little visibility and unclear profile of mathematical chemistry. The second condition brings the field in line with the pluralist and pragmatist methodology of general chemistry, which has, unlike mathematical physics, always preferred developing specific models, rather than universal theories, to address particular issues.

An interesting feature of many HYLE papers, which affects the definition of the subject, is the frequently implicit distinction between mathematical chemistry and discrete mathematical chemistry. The issue is particularly discussed in Klein's paper[9], arguing that several definitions of mathematical chemistry focus only on some particular branches of discrete mathematics, e.g. graph theory. Klein's view is evidenced by the contributions of Hosoya[23], Basak[24] and Balaban[26], which are mainly devoted to the advantage of implementing elements of graph theory in chemistry.

The question arising here is whether only some particular branches of mathematics are suitable to cope with chemical knowledge and its underlying ontology. Ugi and co-

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[iii] While writing this document, Martin Karplus, Michael Levitt and Arieh Warshel were awarded the 2013 Nobel prize in chemistry "for the development of multiscale models for complex chemical systems", which can be regarded as an instance of the fruitful relationship between mathematics and chemistry.

workers[10] and Rouvray[27,28] claimed already in the 1970s that topology, group, graph and category theories are of special importance for chemistry. While most of these mathematical branches are indeed discussed in the HYLE papers, category theory has not yet been further explored. Moreover, will model theory, logic, field theory, commutative algebra and game theory, to name but a few other branches of mathematics, play an important role in formalising chemical knowledge in the future? Or will entirely new mathematical theories and fields emerge out of mathematical chemistry? If there are indeed fields of mathematics that are not suitable for chemistry, does that tell us something about chemistry in general and mathematical chemistry in particular?[29]

A particular ontology?

One of the questions we asked in the call for papers for the HYLE issues was whether mathematical chemistry requires specific ontological or metaphysical assumptions regarding the (mathematical) constitution of the world or the reality of mathematical entities[29]. In this respect, Robert J. Deltete[30] discusses the limits of the energetic theory of 19th-century mathematician Georg Helm. In his *Grundzüge der mathematischen Chemie* (Outline of Mathematical Chemistry) of 1894, Helm tried to mathematize chemistry by referring to energy and other thermodynamic functions rather than to atoms and molecules or, more generally, to a materialist ontology. Even though Deltete shows several technical drawbacks of Helm's approach, the paper makes one ponder on whether mathematical chemistry actually requires the ontology of current mainstream chemistry based upon discrete objects like electrons, molecules and atoms. Does mathematical chemistry require or induce an ontological shift in chemistry towards abstract mathematical objects, similar to the historical shift from substances to atoms and molecules?

Kostas Gavroglu and Ana Simões in their HYLE paper[18] discuss the ontological status of fugacity and activity, first introduced by Gilbert Newton Lewis, and of electronic resonance by Linus Pauling. All three concepts were developed within mathematical theories of chemistry, which raises the general question if such theoretically postulated values and entities correspond to anything in reality. And further, if the acceptance of the mathematical theories by chemists depends on their belief in the reality of the corresponding theoretical entities. From their historical case studies the authors conclude that, even if the ontological status of such theoretical entities continued to be debated, the majority of chemists accepted and introduced them as part of the chemical culture and practice, because they were useful in their daily work.

Hosoya[23], Basak[24] and Balaban[26] discuss the importance of molecular descriptors in characterising molecular structures and the different uses they have found. Are those numerical descriptions of molecules shifting the ontology of molecules? Are chemists and mathematical chemists accepting molecular descriptors only because they work well in their models and help them to estimate properties of substances, or do they believe that descriptors have a correspondence in reality? Are chemists ready to replace mechanistic interpretations by abstract mathematical interpretations? Are there more *chemical* mathematical interpretations than physical (mechanical or quantum mechanical) interpretations? Is chemistry ready to shift its ontology further to a non-numerical one based on relations? There is a discussion on the ontological reduction of chemistry to physics – will mathematical chemistry provoke another one about the reduction of chemistry to mathematics?

Mathematical chemistry in action

Schummer[25] deals with methodological issues of mathematical chemistry when discussing seven pitfalls that one should avoid if one wants to rationalise chemical knowledge. The first pitfall is empirical ignorance, i.e. mathematical chemists should be aware of the huge and growing experimental knowledge that their generalisations must not conflict with. If such data are missing, mathematical formalisations are prone to aesthetic guidance, i.e. the search for simple or "beautiful" solutions, which might easily turn into oversimplification and blindness for the complexity of chemical phenomena. Other pitfalls include the fascination with "numerology", the overproduction of numerical results that provide no explanatory insight, the confusion of computation with experimentation as in "computer experiments", and the blind conduct of statistical correlations.

The author also points to the necessity of developing mathematical approaches that are comprehensible for mainstream chemists. Here the community of mathematical chemists need to develop communicative and translational skills that support the understanding and use of their approaches and results. As an example, Gavroglu and Simões[18] discuss how the abstract concepts of fugacity and activity by Lewis were transmitted and adjusted to the problems and needs of experimental chemists. Likewise, Pauling's efforts of spreading the concept of resonance in mainstream chemistry were so successful that it eventually became a standard part of organic chemistry textbooks.

Next generation

The popularisation of mathematical chemistry is still unsatisfactory. Although there are now several anthologies, for which Denis H. Rouvray has played an important editorial role, and journals devoted to mathematical chemistry; there is no single textbook addressing chemistry students or non-mathematical chemists. That is a task the community needs to tackle, which is certainly difficult to attain because of the diversity of approaches, but utterly important for the broader acceptance of the discipline.

Rouvray mentioned in 1973[27] that the first book devoted to the training of chemists in mathematics (rather than to the popularisation of mathematical chemistry), was Mellor's *Higher Mathematics for Students of Chemistry and Physics*[31], published in 1902. The book provides introductions to differential and integral calculus, analytical geometry, functions, infinite series, numerical methods, differential equations, Fourier's theorem, probability, calculus of variations and determinants. Nowadays there are several other books, e.g. *Maths for Chemistry: A chemist's toolkit of calculations*[32] and *The*

Chemistry Maths Book[33], which largely include the same topics as Mellor's. *Mathematics for Chemistry & Physics*[34] adds group theory to that list. However, themes like point-set topology, category theory, graph theory, network analysis, information theory, order theory, to name but a few that matter in mathematical chemistry, are missing in all those textbooks.

Historically, many good textbooks in chemistry and other disciplines grew out of lecture notes. If mathematical chemistry follows that path, then a formal class on the subject would be the starting point. As far as we know some mathematical chemists, besides lecturing in mainstream chemistry, also teach specialised courses on topics of mathematical chemistry. That would be an opportunity for drafting a textbook.

In order to ensure the continuity of the discipline, novices are needed who become the next generation of mathematical chemists. Apart from conferences, meetings, symposia and workshops open to the interested public, a more direct strategy to motivate and enrol novices is the organisation of schools of mathematical chemistry where leading scholars give general lectures about their research subjects rather than present their latest results. As mentioned in a recent account[5], "these kinds of schools have the advantage of presenting the students the history and reasons to open a particular subject", and "the questions that motivated its development". There are examples of successful schools of that kind, for instance the *Summer Schools of Quantum Chemistry* organised by Per-Olov Löwdin around 1958 out of which the *International Winter Institutes at Sanibel Island and Gainesville* grew. Although there have been some efforts by Subhash C. Basak and Ante Graovac (who unfortunately recently passed away) to organise schools of mathematical chemistry along with scholarly meetings, like the *Indo-US Lecture Series on Discrete Mathematical Chemistry* and the *MATH/CHEM/COMP* meetings, such schools need to be institutionalised, with support grants ensuring their continuity, and held in different corners of the globe to spread mathematical chemistry widely.

Another way of recruiting novices is by directly influencing the chemistry curriculum at universities. That requires mainstream chemists being convinced of the advantages of the mathematical way of thinking in chemistry. It also implies close contact and discussion with scholars involved in curricula development on the local, national and international level. A first step in that direction would be attending meetings on chemical education to promote the need of a broader mathematical training for chemists. This is something the mathematical chemistry community should undertake as one of its programmes. Quoting again Comte, "the perfection of chemistry might be secured and hastened by the training of the minds of chemists in the mathematical spirit"[19].

Social aspects

Several papers comment on the social aspects of mathematical chemistry. For instance, Schummer[25] argues that mathematical chemistry cannot be compared with mathematical physics, because the latter historically emerged out of a single tradition (that of mathematics), whereas the former requires bridging two different cultures (that of chemistry and mathematics). Taking into account that the consolidation of mathematical chemistry began in the second half of the 20^{th} century with approaches to chemistry from discrete mathematics, Restrepo and Villaveces[13] explore the reasons for the institutionalisation of the discipline particularly in Eastern Europe. They conclude that the institutionalisation took place in that region mainly because of the availability of mathematical knowledge among chemists and the lack of research funds for expensive instrumentation. Still an open question is if the development of discrete mathematical chemistry with its focus on graph theory was related to the particular education in that region.

Basak[24] shows how the formalisation of molecular structure has led to a close contact with the chemical industry, particularly the pharmaceutical one, since graph theory and statistics have played an important role in drug discovery and toxicology. Could such interactions be extended to other industrial branches? Or, is one industrial sector benefiting more than others from mathematical chemistry for methodological reasons?

A related issue, not dealt with in the HYLE papers, is the kind of support received by mathematical chemists to pursue their researches. Is the dynamics of funding more akin to the dynamics of mathematics or to that of chemistry? Is mathematical chemistry mainly funded by universities and academic institutions or, in contrast, by the private sector, and how does that affect the research dynamics? Are there industrial spin-offs emerging from mathematical chemistry? A partial answer to this question has been given for chemoinformatics, where several companies fund research projects and where some researchers have founded start-ups[35]. Are there other examples, different from chemoinformatics? If there are more industrial sectors interested in mathematical chemistry, are they willing to support the aforementioned schools of mathematical chemistry? Because some of these questions can easily be addressed by scientometric methods, the mathematical chemistry community would do well to undertake a corresponding research project as part of the discipline and its self-understanding.

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The papers of the special issue of HYLE deal with a broad spectrum of historical, philosophical and social issues regarding mathematical chemistry and, more generally, the relationship between mathematics and chemistry. They raise questions that are usually not asked in the daily research practice, even though they are important for the broader understanding and flourishing of a discipline. By no means do they exhaust the material, but should rather be understood as a starting point and an invitation for further research and discussion. However, they proof that mathematical chemistry is an extremely interesting field of study not only for chemists and mathematicians but also for philosophers and historians of science.

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