Editorial Introduction
Chemistry and Mathematics, Part I

Guillermo Restrepo and Joachim Schummer

The appearance of three scientific journals devoted to mathematical chemistry, the foundation of an academy of mathematical chemistry, various books on the subject as well as regular conferences all testify to the establishment of an international community of mathematical chemistry since the mid-20th century and a new subdiscipline, according to standard criteria of discipline formation.

Philosophers of the past, particularly Kant and Comte, have pondered on the relationship between mathematics and chemistry, usually pointing out their radically different epistemologies. It is perhaps the distinction between *a priori* and *a posteriori* knowledge, which both research fields each appear to exemplify, that kept mathematicians and chemists largely apart from each other, which contrasts with the early establishment of mathematical physics. The delay suggests possible epistemological barriers between the two fields, which philosophical and historical analysis might help understand and perhaps eventually overcome.

From the received mainstream philosophy of science point of view, which was largely a philosophy of mathematical physics, the mathematization of science was simply taken for granted. That there could be barriers in the real sciences, not only in chemistry but also in biology among others, was beyond the horizon. As the aim of this journal is to contemplate on philosophical issues of chemistry that are pressing in the field, regardless of whether they are mainstream or not, the mathematization of chemistry deserves particular attention.

To that end, we have invited both scholars working in mathematical chemistry and philosophers and historians of chemistry to reflect on the interaction between mathematics and chemistry (see our Call for Papers). The numerous positive responses and their different orientation have encouraged us to divide this special issue into two parts. The first part, published in this issue, deals with the relationships between mathematics and chemistry both historically and in general, whereas the second part will particularly investigate the current discipline of mathematical chemistry.

The introductory paper by GUILLERMO RESTREPO and JOSÉ L. VILLAVECES, 'Mathematical thinking in chemistry', provides a broad overview of

HYLE – International Journal for Philosophy of Chemistry, Vol. 18 (2012), No.1, 1-2.
Copyright © 2012 by HYLE and Guillermo Restrepo & Joachim Schummer

the early history of mathematics in chemistry, dating back to Plato, in order to oppose the frequent view that mathematical chemistry as a research field would have emerged only in the 20th-century. The authors suggest a general definition for mathematical chemistry based upon the mathematical way of thinking established in the 19th-century Erlangen Program by mathematician Felix Klein.

In the second paper, 'Georg Helm's chemical energetics', ROBERT J. DELTETE discusses the limits of the energetic theory of the 19th-century German mathematician Georg Helm. In his *Grundzüge der mathematischen Chemie: Energetik der chemischen Erscheinungen* (The Principles of Mathematical Chemistry: The Energetics of Chemical Phenomena) from 1894, which can also be read as a textbook of chemical thermodynamics, Helm tried to mathematize chemistry in contrast to contemporary atomistic accounts of chemistry. In that approach, mathematics appeared as an antidote to metaphysics in chemistry or at least as a means to minimize ontological claims.

In 'From physical chemistry to quantum chemistry. How chemists dealt with mathematics' KOSTAS GAVROGLU and ANA SIMÕES investigate the subsequent 20th-century mathematization of chemistry by two case studies: Lewis' introduction of fugacity and activity into chemical thermodynamics and Pauling's concept of resonance in quantum chemistry. They argue that the mathematization of chemistry raised not so much methodological issues among chemists but, contrary to Helm's case, suggested new kinds of theoretical entities and quantities whose ontological status were heavily debated.

In 'Why mathematical chemistry cannot copy mathematical physics and how to avoid the imminent epistemological pitfalls' JOACHIM SCHUMMER points out fundamental historical and methodological differences between mathematical chemistry and mathematical physics, such the latter cannot simply imitate the former. To distinguish mathematical chemistry from both mathematical physics and physical chemistry, he suggests a methodological definition of the field and then highlights obvious epistemological pitfalls that are illustrated by historical cases and which can be avoided only through strong ties with experimental chemists.

Finally, we are very happy to include a book review of *Neither Physics Nor Chemistry: A History of Quantum Chemistry* (2012) by Kostas Gavroglu and Ana Simões, written by eminent quantum chemist BRIAN T. SUTCLIFFE who had first-hand experience of most of that history.

We really hope that this and the forthcoming issue of HYLE will encourage further in-depth discussion of the much neglected relationship between chemistry and mathematics.