Editorial
Mathematics and Chemistry, Part II

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Between mathematics, the deductive science *par excellence*, and chemistry, which has long been the epitome of the experimental laboratory science, the epistemological differences can hardly be overestimated. The first part of this special issue on 'Mathematics and Chemistry' (HYLE, vol. 18, no. 1) has focused on general aspects and the early history of their relationships, the methodological barriers as well as various attempts at mathematizing chemistry. The present part is devoted to the institutionalization of that relationship in the form of the discipline of mathematical chemistry, both as a distinctive field of study and a scientific community that emerged in the second half of the 20th century. We are delighted to present five contributions from leading members of mathematical chemistry, of which some were indeed extremely influential in establishing and shaping that discipline.

In the first paper, 'Philosophy of mathematical chemistry: a personal perspective', SUBHASH C. BASAK provides an excellent introduction to important parts of discrete mathematical chemistry. Illustrated with examples from his own research, he explains how molecules and macromolecules can be represented by graphs and matrices to attain models that quantify several molecular features and properties. He further shows how mathematical chemistry has become an active scientific field with both basic and applied research and with connections to the chemical and pharmaceutical industries.

In 'Discrete mathematical chemistry, social aspects of its emergence and reception', GUILLERMO RESTREPO and JOSÉ L. VILLAVECES investigate the social conditions that favored the origin of the field in the second half of the 20th century and which hindered its later development. They claim that the field arose largely in Eastern Europe because of both the availability of mathematical knowledge among chemists and the lack of research funds. The authors further argue that discrete mathematical chemistry was flatly rejected by many chemists and only slowly accepted in mathematics. Finally they suggest a definition of the subject that makes use of ideas from August Comte and Hermann Weyl, thereby discarding the notion that mathematical chemistry would simply be mathematics applied to chemistry.

While the first two papers focus on discrete mathematical chemistry, which employs mathematics of noncontinuous structures, DOUGLAS J.

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KLEIN, in 'Mathematical chemistry! Is it? And if so, what is it?', takes a broader perspective. He defines mathematical chemistry as the development of novel mathematics whatsoever for chemical applications, for which he finds a long and rich history in 25 different research areas of chemistry. He argues that mathematical chemistry was only recently recognized as an own field because before it was frequently regarded as a part of physical chemistry, or the often 'non-numerical' mathematics involved was not recognized as mathematics. Finally he defends the identity of mathematical chemistry by discussing its relationships to physical chemistry, computational chemistry, and theoretical chemistry.

Klein's notion that mathematical chemistry develops novel mathematics implies a reverse impact on the advancement of mathematics. In 'What can mathematical chemistry contribute to the development of mathematics?', HARUO HOSOYA illustrates such an impact from his own pioneering work. Assuming that abstract chemical thinking differs not essentially from that of mathematics but seeks visualization in graphs and structural formulas, he shows how the Z-index, which was developed to describe molecular structures, can help visualize and further develop abstract features of mathematical number theory. His second example provides insight in how group theoretical reasoning in fullerene chemistry advanced the mathematical theory of regular polyhedra.

Finally, in 'Chemical graph theory and the Sherlock Holmes principle', ALEXANDRU T. BALABAN provides a personal perspective on chemical applications of graph theory, where he has played an eminent role. He compares his research strategy to tackle chemical questions through graph theory with the 'Sherlock Holmes principle' of eliminating impossible solutions through further analysis. In an autobiographical account he describes his involvement in various research fields (including isomer enumeration, mathematical treatment of chemical reactions, molecular characterization, and the mathematics of fullerenes and nanostructures) not without considering the social and political conditions of the time.

We hope that this second issue of HYLE dedicated to the relationship between mathematics and chemistry encourages further discussion on the subject as there are still open questions. In particular, the delayed reception of mathematical chemistry by bench chemists calls for deeper philosophical analysis, because that was likely caused by different ideas about what a theory in chemistry is and should provide, what a convincing explanation, a reliable prediction, and a sound justification is, and more generally about what the epistemological and ontological foundations of chemistry are.

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