BOOK REVIEW

CHEMISTRY AND MATHEMATICS: TWO SCIENTIFIC LANGUAGES OF THE 21st CENTURY

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This publication may be viewed as an issue of *Nova Acta Leopoldina,* in particular its number 330 and volume 88, but (as this reviewer prefers) also as a separate book. Anyway, it contains papers presented at a scientific conference, held in Göttingen on October 11 to 13, 2001, under the auspices of the German Academy of Natural Sciences Leopoldina, the Göttingen Academy of Sciences, and the French Academy of Sciences, The book contains 8 articles (that this reviewer will refer to as chapters), preceded by in introduction written by Herbert W. Roesky,

In the *"Introduction"* (pp. 7–9) Roesky recalls that *a language is a system of verbal signs which are typical for a community of people who want to express what they think and who want to be understood by the other members of the community.* Because *modern chemistry and mathematics began... to discover that there are a lot of things they share,* the purpose of this conference was to bring chemists and mathematicians together, in order that they could better understood each other. This is best expressed by Peter Deuflhard, who, by studying the relations of the scientific languages of chemistry and mathematics, concludes: *The common clear message from these comparisons is that chemical intuition may pave the way for mathematical concepts just as chemical concepts may gain from mathematical precisioning. Along this line, significant improvements in chemical research and engineering have already been possible – and can be further expected in the future from the dialogue between the two scientific languages.*

The first chapter is *"Chemistry as an Ideographic Language"* by Guy Ourisson (pp. 11-18). It briefly outlines the wealth of information contained in a structural formula of an organic compound. What the paper does not mention is that such formulas have also a mathematical content, recognized already in the middle of the 19th century.

The second chapter "*Transition Metal-Based Machines and Motors at the Molecular Level"* (pp. 19–38) is written by Jean-Paul Collin and four coauthors. It contains

exactly what the title says and is nothing but a well–written (chemical) review article.

The next chapter is *"Virtual Crystallography"* by Olaf Delgado-Friedrichs (pp. 39–49). It describes the author's original and interesting combinatorial and geometric researches, related to crystallography.

Follows "*A Comparison of Related Concepts* in *Computational Chemistry and Mathematics"* by Peter Deuflhard (pp. 51–66). This text goes to the very center of the theme. It considers three mathematical concepts (intrinsic low-dimensional manifolds, Galerkin's method for constructing special Hilbert spaces, and geometrical conformations) and connects them with three fields of physico-chemical research (quasi-stationary state approximation in chemical kinetics, lumping in polymer kinetics, and molecular conformational analysis).

The fifth chapter "*The Essence of Chemical Thinking Beyond Mathematical Equations"* by Jerzy Haber (pp. 67–80) has the ambition to demonstrate that *chemistry is based* on *an interplay of theory, comprising phenomenological inductive laws and deductive theory, experiments, and chemical intuition,* and that *chemistry developed its own ideographic language, whose semiotic rules permit to understand reaction mechanisms.* In spite of these abstract claims, the article mainly outlines the author's own (experimental) research of catalytic oxidation of hydrocarbons. A few philosophical thoughts are found only at the end of the text, whereas mathematics is completely absent.

The next chapter is *"Analysis of Chemical Reaction Systems – What Are Mathematics Able to Do, How Far Has Chemistry to Help?"* by Jürgen Warnatz (pp. 81–108). It provides examples for how complex phenomena encountered in chemical and industrial processes are modelled by mathematical methods. These will be found interesting by both chemists and mathematicians.

The *"Poetic Suggestion in Chemical Science"* (pp. 109–139), written by (Sir) John Meurig Thomas, expresses some thoughts on the artistic and poetic aspects of both mathematics and chemistry, richly illustrated by facts and pictures from their past and present. Although the entire book is full of high-quality and beautiful figures, this chapter is really a piece of art. It would be good to make this article available to high-school students, before they decide what they will be studying – the number of those choosing chemistry would increase significantly.

The last chapter *"Combustion: From Mathematical Models to Practical Devices",* by Jürgen Wolfrum (pp. 141–160), is a fine survey of the physical chemistry of combustion, however with very few details on its mathematical modelling.

There is a total of 218 references quoted in this book. Not a single one is from the *Journal of Mathematical Chemistry* or *MATCH Communications in Mathematical and in Computer Chemistry,* the only two journals devoted to mathematics-related researches in chemistry. Not a single quotation is from the *Journal of Computational Chemistry* or *Journal of Chemical Information and Computer Sciences* or *Computers & Chemistry,* the three main journals for publishing computer-aided researches in chemistry. Not a single quotation is from *Theoretical Chemistry Accounts* (former

Theoretica Chimica Acta) or *International Journal of Quantum Chemistry,* the leading journals for theoretical chemistry. This says something about the modes by which the authors of the book were invited or selected, and the connection of the contents of the book to contemporary scientific activities, lying on the border between mathematics and chemistry, sometimes referred to as *Mathematical Chemistry.*

In spite of the above, there is no doubt that the book "*Chemistry and Mathematics: Two Scientific Languages of the* 21st *Century"* is a valuable attempt to improve understanding, communication, and cooperation between mathematicians and chemists. From a technical point of view, the book is a masterpiece.

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