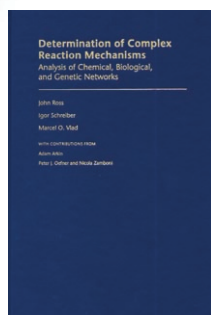




Determination of Complex Reaction Mechanisms



Analysis of Chemical, Biological, and Genetic Networks. By John Ross, Igor Schreiber, and Marcel O. Vlad. Oxford University Press, Oxford 2005. 226 pp., hardcover \$ 94.50.—ISBN 0-19-517868-8

The last decades have seen a remarkable advancement in our understanding of molecular and supramolecular structures in chemistry, materials science, and biology. While these advances have undoubtedly enjoyed the limelight, surprising and profound progress has also occurred in the field of chemical kinetics. The book *Determination of Complex Reaction Mechanisms*, by Ross, Schreiber, and Vlad, describes some of these achievements in the form of a 226-page treatise. It is worth mentioning that John Ross, Professor Emeritus at Stanford University and 1999 National Medal of Science laureate, has been for decades one of the leading figures in this field. Together with Berry and Rice, he also authored a well-known textbook on physical chemistry.

Determination of Complex Reaction Mechanisms assumes a basic knowledge of chemical kinetics. However, the way that it approaches chemical kinetics is highly unconventional, interesting, and useful. The key question behind most of this book is “How do I unravel the mechanism of a complex chemical, biochemical, or genetic reaction network?”

Conventional approaches today seem to differ only slightly from the way our grandparents would have attacked the problem, namely: 1) break down the complexity of the system by isolating and characterizing individual reaction steps, and 2) propose a reaction mechanism constructed from a reasonable sequence of elementary steps. The approach presented in *Determination of Complex Reaction Mechanisms* is profoundly different. It is based on the simple fact that today chemists are equipped with a powerful arsenal of analytical techniques. These techniques allow the simultaneous monitoring of hundreds of different chemical species, thus providing an enormous amount of data regarding the full reaction mechanism. The main value of this book is that it discusses experimental protocols and theoretical methods for the rational elucidation of reaction networks and their kinetic parameters by utilizing such techniques. In other words, it is a manual that describes nontraditional methodologies for the determination of reaction mechanisms from kinetic data sets.

The book is organized in 13 chapters, and also contains contributions from Arkin, Oefner, and Zamboni. Following a very brief introduction of basic terms and definitions, Chapter 3 reviews some of the data-mining methodologies suitable for the analyses discussed in this book. These methodologies range from mass spectrometry and capillary electrophoresis to DNA microarrays and genome-wide analyses of mRNA and proteins. Specific types of data analysis are presented in the main part of the book. Chapter 5, for example, discusses the response of complex systems to pulse perturbations, from which causal chemical connectivities can be derived. This interesting chapter starts with the analysis of simple unbranched chain reactions, and leads into an experimental case study, a part of glycolysis, which is discussed in Chapter 6. This example is examined further in the discussion of “correlation metric construction” of reaction mechanisms, which I consider to be very exciting. The central aim of this technique is to yield reaction diagrams similar to those that a chemist would draw for complex mechanisms, or at least to indicate the pres-

ence of separable subsystems. Other techniques discussed include applications of entropy metric construction, entropy reduction methods, and genetic algorithms.

The main merit of the approach described is that it addresses one of chemistry’s key questions: how to derive a reaction mechanism without relying on educated guesses and on “chemical intuition”, which although sometimes powerful is often misleading. Specifically, the book provides intriguing tools that might be applicable to many complex systems in the various modern branches of chemistry and biology. However, it should be clearly stated that these tools have been tested for only a few examples. The topics covered are essentially a compilation of the remarkable results obtained by the authors during the last 15 years. However, the book is definitely more than a collection of loosely connected research articles. The authors make a serious, and in my opinion successful, effort to present complex and unconventional topics in a coherent, interesting, and useful way. How quickly this powerful approach will be embraced by a large number of experimentalists remains to be seen. This brings me to the question: who is the intended reader? Clearly, to appreciate this book the potential reader should have a solid background in elementary statistics, linear algebra, and calculus. Those who want to use the techniques described should also be willing to write their own computer codes. Beyond that, I can envision a broad readership, which ranges from graduate students in physical and biophysical chemistry to senior scientists in other fields who face the notorious problem of determining reaction mechanisms or similar network features for complex chemical, biochemical, pharmaceutical, or genetic systems.

Oliver Steinbock
Department of Chemistry and
Biochemistry
Florida State University
Tallahassee (USA)

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