Determination of Complex Reaction Mechanisms: Analysis of Chemical, Biological, and Genetic Networks

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In a chemical system with many chemical species several questions can be asked: what species react with other species: in what temporal order: and with what results? These questions have been asked for over one hundred years about simple and complex chemical systems, and the answers constitute the macroscopic reaction mechanism. In Determination of Complex Reaction Mechanisms authors John Ross, Igor Schreiber, and Marcel Vlad present several systematic approaches for obtaining information on the causal connectivity of chemical species, on correlations of chemical species, on the reaction pathway, and on the reaction mechanism. Basic pulse theory is demonstrated and tested in an experiment on glycolysis. In a second approach, measurements on time series of concentrations are used to construct correlation functions and a theory is developed which shows that from these functions information may be inferred on the reaction pathway, the reaction mechanism, and the centers of control in that mechanism. A third approach is based on application of genetic algorithm methods to the study of the evolutionary development of a reaction mechanism, to the attainment given goals in a mechanism, and to the determination of a reaction mechanism and rate coefficients by comparison with experiment. Responses of non-linear systems to pulses or other perturbations are analyzed, and mechanisms of oscillatory reactions are presented in detail. The concluding chapters give an introduction to bioinformatics and statistical methods for determining reaction mechanisms.

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