



# Chemical Graph Theory: Reactivity and Kinetics (Mathematical Chemistry)

*Danail Bonchev*

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## **Chemical Graph Theory: Reactivity and Kinetics (Mathematical Chemistry)** Danail Bonchev

This volume is concerned with applications of graph theory to the study of chemical kinetics and reaction mechanisms. Methods of handling kinetic data are explained with emphasis on the derivation of rate laws and related problems. Graph-based classification and coding of reaction mechanisms along with approaches for determining their complexity are described, providing researchers with a useful tool in their search for new reaction mechanisms. The operator set approach to the structural and dynamic interrelations between chemical species is presented as a methodology for discovering new selection and prohibition rules. Also discussed are the reaction lattice technique and its application to aromaticity and pericyclic reactions, and the DARC/PELCO method, a topological tool for QSAR searching.

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