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Sommario/riassunto

Providing an overview of the latest computational approaches to estimate rate constants for thermal reactions, this book addresses the theories behind various first-principle and approximation methods that have emerged in the last twenty years with validation examples. It presents in-depth applications of those theories to a wide range of basic and applied research areas. When doing modeling and simulation of chemical reactions (as in many other cases), one often has to compromise between higher-accuracy/higher-precision approaches (which are usually time-consuming) and approximate/lower-preci