



Rate Constant Calculation for Thermal Reactions: Methods and Applications

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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-precision approaches (which often has the advantage of speed in providing results). This book covers both approaches. It is augmented by a wide-range of applications of the above methods to fuel combustion, unimolecular and bimolecular reactions, isomerization, polymerization, and to emission control of nitrogen oxides. An excellent resource for academics and industry members in physical chemistry, chemical engineering, and related fields.

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