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2.7 Peroxy radical isomerization2.8 Theoretical and dynamical studies of the hydrogen/oxygen system; References; Chapter 3. Kinetics databases; 3.1 Data for combustion modelling; 3.2 Primary sources of kinetic data: the need for evaluation; 3.3 Evaluation of kinetic data; 3.4 Interpolation, extrapolation and estimation procedures; 3.5 Data sources for modelling; References; Chapter 4. Mathematical tools for the construction, investigation and reduction of combustion mechanisms; 4.1 Introduction; 4.2 Notation; 4.3 The construction of combustion mechanisms
4.4 Numerical investigation of complex models4.5 Sensitivity and uncertainty analysis; 4.6 Mechanism reduction without time-scale analysis; 4.7 Formal lumping procedures; 4.8 Reduction based on the investigation of time-scales; 4.9 Approximate lumping in systems with time-scale separation; 4.10 Fitted kinetic models; 4.11 Conclusions and future directions; Chapter 5. Global behaviour in the oxidation of hydrogen, carbon monoxide and simple hydrocarbons; 5.1 Introduction; 5.2 Notation; 5.3 Non-linearity and feedback in chemical kinetics: stoichiometry and elementary steps
5.4 Chemical feedback: branched-chain ignition5.5 Thermal feedback: ignition, extinction and singularity theory; 5.6 Thermokinetic feedback: oscillations and local stability analysis; 5.7 The H2 + O2 reaction: p-Ta ignition limits in closed vessels; 5.8 Flow reactor studies of the H2 + O2 reaction; 5.9 Complexity in the oscillatory ignition region; 5.10 Mechanistic modelling of complexity in the H2 + O2 reaction; 5.11 The CO + O2 reaction; 5.12 Hydrocarbon oxidation; 5.13 Conclusions and future directions; References
Chapter 6. Experimental and numerical studies of oxidation chemistry and spontaneous ignition phenomena

Sommario/riassunto

Combustion has played a central role in the development of our civilization which it maintains today as its predominant source of energy. The aim of this book is to provide an understanding of both fundamental and applied aspects of low-temperature combustion chemistry and autoignition. The topic is rooted in classical observational science and has grown, through an increasing understanding of the linkage of the phenomenology to coupled chemical reactions, to quite profound advances in the chemical kinetics of both complex and elementary reactions. The driving force has been both the intrinsic