1. Record Nr. UNISA996197710203316

Titolo	The investigation of organic reactions and their mechanisms [[electronic resource] /] / edited by Howard Maskill
Pubbl/distr/stampa	Oxford ; ; Ames, Iowa, : Blackwell Pub., 2006
ISBN	1-281-32018-8 9786611320188 0-470-98867-3 0-470-99416-9 0-470-76261-6
Descrizione fisica	1 online resource (394 p.)
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Disciplina	547.2 547/.2
Soggetti	Physical organic chemistry Chemical reactions Chemical processes
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	The Investigation of Organic Reactions and Their Mechanisms; Contents; Contributors; Foreword; Preface; 1 Introduction and Overview; 1.1 Background; 1.2 The nature of mechanism and reactivity in organic chemistry; 1.3 The investigation of mechanism and the scope of this book; 1.3.1 Product analysis, reaction intermediates and isotopic labelling; 1.3.1.1 Example: the acid-catalysed decomposition of nitrosohydroxylamines; 1.3.2 Mechanisms and rate laws; 1.3.3 Computational chemistry; 1.3.3.1 Example: the acid- and base-catalysed decomposition of nitramide; 1.3.4 Kinetics in homogeneous solution 1.3.4.1 Example: the kinetics of the capture of pyridyl ketenes by n -butylamine1.3.5 Kinetics in multiphase systems; 1.3.6 Electrochemical and calorimetric methods; 1.3.7 Reactions involving radical intermediates; 1.3.8 Catalysed reactions; 1.4 Summary; Bibliography; References; 2 Investigation of Reaction Mechanisms by Product Studies; 2.1 Introduction and overview- why study organic reaction

mechanisms?; 2.2 Product structure and yield; 2.2.1 Quantitative determination of product yields; 2.2.2 Product stabilities, and kinetic and thermodynamic control of product formation
2.3 Mechanistic information from more detailed studies of product structure2.3.1 Stereochemical considerations; 2.3.2 Use of isotopic labelling; 2.4 Mechanistic evidence from variations in reaction conditions; 2.5 Problems and opportunities arising from unsuccessful experiments or unexpected results; 2.6 Kinetic evidence from monitoring reactions; 2.6.1 Sampling and analysis for kinetics; 2.7 Case studies: more detailed mechanistic evidence from product studies; 2.7.1 Product-determining steps in SN1 reactions; 2.7.2 Selectivities; 2.7.3 Rate- product correlations; Bibliography; References
3 Experimental Methods for Investigating Kinetics3.1 Introduction; 3.2 Preliminaries; 3.2.1 Reaction rate, rate law and rate constant; 3.2.2 Reversible reactions, equilibrium and equilibrium constants; 3.2.3 Reaction mechanism, elementary step and rate-limiting step; 3.2.4 Transition structure and transition state; 3.3 How to obtain the rate equation and rate constant from experimental data; 3.3.1 Differential method; 3.3.1.1 Example:reaction between RBr and HO-; 3.3.2 Method of integration; 3.3.2.1 Data handling; 3.3.2.2 Example: decomposition of N2O5 in CCl4; 3.3.3 Isolation method
3.3.3.1 Example: oxidation of methionine by HOCl3.4 Reversible reactions and equilibrium constants; 3.4.1 Rate constants for forward and reverse directions, and equilibrium constants; 3.4.1.1 Example: cis-trans isomerisation of stilbene; 3.5 Experimental approaches; 3.5.1 Preliminary studies; 3.5.2 Variables to be controlled; 3.5.2.1 Volume; 3.5.2.2 Temperature; 3.5.2.3 pH; 3.5.2.4 Solvent; 3.5.2.5 Ionic strength; 3.5.2.6 Other experimental aspects; 3.6 Choosing an appropriate monitoring method; 3.6.1 Periodic monitoring; 3.6.2 Continuous on-line monitoring; 3.6.3 Continuous static monitoring
3.7 Experimental methods

Sommario/riassunto

A range of alternative mechanisms can usually be postulated for most organic chemical reactions, and identification of the most likely requires detailed investigation. Investigation of Organic Reactions and their Mechanisms will serve as a guide for the trained chemist who needs to characterise an organic chemical reaction and investigate its mechanism, but who is not an expert in physical organic chemistry. Such an investigation will lead to an understanding of which bonds are broken, which are made, and the order in which these processes happen. This information and knowledge of the a