

1. Record Nr.	UNINA9910146086703321
Titolo	Quinone methides [[electronic resource] /] / edited by Steven E. Rokita
Pubbl/distr/stampa	Hoboken, N.J., : Wiley, 2009
ISBN	1-282-68959-2 9786612689598 0-470-45288-9 0-470-45287-0
Descrizione fisica	1 online resource (460 p.)
Collana	Wiley series on reactive intermediates in chemistry and biology
Altri autori (Persone)	RokitaSteven Edward
Disciplina	547.2 547/.2
Soggetti	Intermediates (Chemistry)
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	QUINONE METHIDES; CONTENTS; Preface to Series; Introduction; Contributors; 1 Photochemical Generation and Characterization of Quinone Methides; 1.1 Introduction; 1.2 Quinone Methides from Benzylic Photoelimination; 1.2.1 Photoelimination of Fluoride; 1.2.2 Photodehydration; 1.2.3 Photoelimination of Quaternary Ammonium Salts; 1.2.4 Photoelimination of Alcohols and Esters; 1.3 Quinone Methides from ESIPT to Unsaturated Systems; 1.3.1 Quinone Methides from ESIPT to Carbonyls; 1.3.2 Quinone Methides from ESIPT to Alkenes and Alkynes; 1.3.3 Quinone Methides from ESIPT to Aromatic Carbon 1.4 Other Photochemical Routes to Quinone Methides1.5 Conclusions and Outlook; References; 2 Modeling Properties and Reactivity of Quinone Methides by DFT Calculations; 2.1 Introduction; 2.2 QM Reactivity as Alkylating Agents; 2.2.1 Computational Models; 2.2.1.1 Basis Set Choice; 2.2.1.2 Energetics of the Benzylation by o-QM in the Gas Phase and in Aqueous Solution; 2.2.2 H-Bonding and Solvent Effects in the Benzylation of Purine and Pyrimidine Bases; 2.2.2.1 Cytosine Benzylation under Kinetic Control; 2.2.2.2 Stability/Reactivity of the QM-Cytosine Conjugates 2.2.2.3 Purine Bases Benzylation: Kinetic and Thermodynamic Aspects2.3 Reactivity as Heterodiene; 2.4 Tautomerizations Involving

Quinones and Quinone Methides; 2.4.1 QM Versus Quinone Stability: Substituent Effects; 2.5 o-Quinone Methide Metal Complexes; 2.5.1 Geometries and Reactivity as Function of the Metal and the Structural Features; 2.6 Generation of o-QM; 2.6.1 Generation of o-QM Tethered to Naphthalene Diimides by Mild Activation; 2.6.2 Thermal Generation of o-QM in Oxidative Processes in the Gas Phase; 2.7 Thermal Decomposition of o-QM in the Gas Phase  
2.8 QM Generation in Lignin Formation  
2.9 Conclusion and Perspective;  
References; 3 Quinone Methide Stabilization by Metal Complexation; 3.1 Introduction; 3.2 QM-Based Pincer Complexes; 3.2.1 Formation; 3.2.2 Reactivity and Modifications; 3.2.3 Os-Based, p-QM Complexes; 3.3 One-Site Coordinated QM Complexes; 3.3.1 (2)-ortho-QM Complexes; 3.3.1.1 Formation; 3.3.1.2 Release and Reactivity of (2)-o-QMs; 3.3.2 (2)-p-QM Complexes; 3.3.2.1 Formation; 3.3.2.2 Controlled Release and Modification of (2)-p-QMs; 3.4 (4)-Coordinated QM Complexes; 3.4.1 Formation of (4)-Coordinated QM Complexes  
3.4.2 Reactivity of (4)-Coordinated QM Complexes  
3.4.3 (4)-Coordinated QM Complexes of Mn; 3.5 Characterization of QM Complexes; 3.5.1 IR; 3.5.2 (1)H and (13)C {(1)H} NMR; 3.5.3 X-Ray; 3.6 Conclusion and Future Applications; Acknowledgments; References; 4 Intermolecular Applications of o-Quinone Methides (o-QMs) Anionically Generated at Low Temperatures: Kinetic Conditions; 4.1 Introduction to o-QMs; 4.2 Thermal Generation Conditions; 4.3 Low-Temperature Kinetic Generation of o-QMs; 4.3.1 Formation of the o-QMs Triggered by Fluoride Ion; 4.3.2 Stepwise Formation of o-QMs  
4.3.3 Kinetically Controlled Cycloadditions

---

## Sommario/riassunto

Multidisciplinary perspectives and approaches to quinone methides research. The Wiley Series on Reactive Intermediates in Chemistry and Biology investigates reactive intermediates from the broadest possible range of disciplines. The contributions in each volume offer readers fresh insights into the latest findings, emerging applications, and ongoing research in the field from a diverse perspective. This inaugural volume in the series, Quinone Methides, represents the first book devoted to this fascinating and useful intermediate. The authors of this work reflect the many disciplines

---