

1. Record Nr.	UNINA9910809459903321
Autore	Zhu Hua-Jie
Titolo	Organic stereochemistry : experimental and computational methods / / Hua-Jie Zhu
Pubbl/distr/stampa	Weinheim an der Bergstrasse, Germany : , : Wiley-VCH Verlag GmbH & Co. KGaA, , 2015 ©2015
ISBN	3-527-68817-X 3-527-68816-1
Descrizione fisica	1 online resource (337 p.)
Disciplina	541.223
Soggetti	Stereochemistry Physical organic 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 at the end of each chapters and index.
Nota di contenuto	Cover; Title Page; Copyright; Contents; Preface; Acknowledgments; List of Abbreviations; Part I Fundamentals; Chapter 1 Chirality; 1.1 Introduction; 1.2 Tetrahedron of Carbon; 1.2.1 Terpenoids; 1.2.2 Flavonoids; 1.2.3 Alkaloids; 1.2.4 Steroids; 1.2.5 Glycosides; 1.2.6 Others; 1.3 Other Stereogenic Centers; 1.4 Optical Characteristics; 1.4.1 Measurement of OR; 1.4.2 ECD and Its Definition; 1.4.3 Outline of VCD; 1.4.4 Outline of ROA; References; Chapter 2 Non-optical Method in Configuration Study; 2.1 ^{13}C NMR Spectra; 2.1.1 NMR and Atomic Structure; 2.1.2 ^{13}C NMR Calculation; 2.1.3 ^1H NMR 2.1.4 ^{13}C NMR Prediction and Conformational Search 2.2 X-Ray Diffraction and Mosher Method; 2.2.1 X-Ray Diffraction; 2.2.2 Mosher Method; 2.3 Transition State Energy and Chirality Selectivity; 2.4 Separation of Chiral Compounds; 2.4.1 Chiral Organic Bases; 2.4.2 Chiral Organic Acids; 2.4.3 Chiral Organic Alcohols; 2.4.4 Others; References; Part II Techniques; Chapter 3 Optical Rotation (Rotatory Dispersion, ORD); 3.1 Introduction; 3.2 Quantum Theory; 3.3 Matrix Model; 3.3.1 Matrix Basis; 3.3.2 Explanation of General OR Characteristics; 3.3.2.1 Sample Calculations 3.3.2.2 Calculated Values in Same Series of Compounds 3.4 ORD; 3.5

Application; 3.5.1 AC Assignment for Mono-Stereogenic Center Compounds; 3.5.2 Matrix Model Application; 3.5.3 AC Assignment for Poly-Stereogenic Center Compounds; 3.5.4 Using ORD Method; References; Chapter 4 Electronic Circular Dichroism; 4.1 Exciton Chirality CD; 4.2 ECD Characteristics for Chiral Metallic Compounds; 4.3 Quantum Theory Basis; 4.4 Principle Using ECD; 4.5 Application; 4.5.1 Procedure to Do ECD; 4.5.2 ECD Application; 5.4.1 VCD Application; 4.5.3 UV Correction; References
Chapter 5 Vibrational Circular Dichroism and Raman Optical Activity5.1 Exciton Chirality; 5.2 Quantum Theory Basis; 5.2.1 VCD and IR; 5.2.2 ROA and Raman Scattering; 5.3 Principles Using VCD and ROA; 5.4 Application; 5.4.2 ROA Application; References; Chapter 6 Combinational Use of Different Methods; 6.1 Tactics to Select Methods; 6.1.1 ^{13}C NMR Methods; 6.1.2 OR and ORD; 6.1.3 Matrix; 6.1.4 ECD; 6.1.5 VCD Method; 6.2 Examples and Discussion; 6.3 Revised Structures; 6.3.1 ORD Method; 6.3.2 Combinational Use of OR and ECD; 6.3.3 VCD and ECD; 6.3.4 Comprehensive Use of OR, ECD, and VCD ReferencesPart III Reactions; Chapter 7 Enantioselective Reaction; 7.1 Enantioselective Addition; 7.1.1 Organic Zn- or Zn-Ti Reagent; 7.1.2 Organic Cu-Zn, Cu-Li Reagent; 7.1.3 Organo-Fe Complexes; 7.1.4 Other Organo-Metallic Complexes; 7.1.5 Organo-Si Reagents; 7.2 Enantioselective Reduction; 7.2.1 Green Chemistry; 7.6.2 Auto-Self Catalysis; 7.3 Enantioselective Oxidation; 7.4 Prediction of ee Using Calculations; 7.5 Catalyst Types; 7.5.1 Amino Alcohols; 7.5.2 Chiral Ligands Containing N-O Group; 7.5.3 Chiral Axial Catalysts; 7.5.4 Solid-Supported Chiral Compounds
7.5.5 Spiral Chiral Compounds
