

## The Encyclopedia of Mass Spectrometry, Volume 1, Theory and Ion Chemistry

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By definition, an encyclopedia is "a comprehensive reference work containing articles on a wide range of subjects or on numerous aspects of a particular field." This first volume of Elsevier's *The Encyclopedia of Mass Spectrometry: Theory and Ion Chemistry* more than meets that definition. This book consists of 13 multi-article chapters with each article separately authored, a Forward by the Editors-In-Chief, a Preface by the Volume Editor, an 8-page list of 90 contributors, and a 68-page 3-column-per-page index. There are 91 articles in the 13 chapters with 3 articles each in the smallest chapters ("Mobilities" — Chapter 7; "Biopolymers" — Chapter 13) and 15 articles in the largest chapter ("Thermochemistry (Methods)" — Chapter 5). A list of the articles along with their authors is provided at the end of this review. The Index is definitely of the caliber that should characterize an encyclopedia and is an example of the detail to which the publishers have gone to make this book a useable reference. The index's description and explanations of its function found on the first page of the index is invaluable to the book as a comprehensive reference.

There has not been a comprehensive work on the theory of mass spectrometry instrumentation and ion chemistry since that of G. P. Barnard (*Modern Mass Spectrometry*; The Institute of Physics: London, 1953); i.e., it is curious that the Barnard book and this volume of Elsevier's *Encyclopedia of Mass Spectrometry* are exactly half a century apart. Many other fine reference works have been written in this span of 50 years, but they all covered much broader topics as the field of mass spectrometry grew at a more than exponential rate or had narrower focuses such as those presented in individual articles in this volume. The theory of the control of motion of gas-phase ions in a vacuum and the chemistry of those ions by themselves or in interactions with other matter had to be pulled from multiple references in many different journals, proceedings of meetings, and a few books dedicated to these fields.

This was a daunting task and made preparation of a course of study of these topics formidable. There was no one place to go to get a good understanding of the "what was happening inside the mass spectrometer." This book definitely fills that void.

The 2 chapters on the theory of ion chemistry (Chapters 1 and 2) with their 9 articles and 400+ citations provide an excellent foundation for a graduate-level course on the subject or a neophyte-researcher's beginning quest into the field. Courses on the interpretation of mass spectra of organic ions should require the reading of Chapters 9 and 10, "Organic Ion Chemistry (Positive) and Organic Ion Chemistry (Negative)," respectively, with their 15 articles. These chapters give the foundation to the understanding as to why ions fragment in the ways they do and provide the tools for fragmentation prediction. The six articles in Chapter 6, "Collisional Activation and Dissociation," will also be of value to those trying to get an understanding of the fragmentation process that takes place in MS/MS.

Chapter 8, "Neutralization, Charge Reversal," will also be of interest with respect to an understanding of the chemistry of organics; however, this will be more esoteric than the subjects usually covered in interpretation courses. Chapter 11 "Solvation and Clusters" brings about a preliminary understanding of one of the complexities seen in atmospheric pressure ionization of analytes in the condensed phase. Again, this is a topic which until now has not had a single point source for information. Data had to be extracted from the literature in an arduous process. The citations in the articles in this chapter will act as a guide to more detailed studies of these topics. Long a subject not well addressed in the traditional mass spectrometry books, ion spectroscopy is covered in enough detail in the 11 articles of Chapter 4 with this name to provide a clear understanding of the fundamentals as well as to the values of these types of studies. The same can also be said for the thermochemistry chapter (Chapter 5). The instrumentation chapter (Chapter 3) also takes a different approach from the traditional mass spectrometry text in that, as pointed out in the Preface, research instruments that do not fall into the category of those usually found in the analytical laboratory are discussed. Some instrument types familiar to the applications analytical chemist such as the ion cyclotron resonance, quadrupole ion trap, and time-of-flight instruments are discussed in this chapter with respect to their operational theory in the vein of their use as tools to study ion physics. Fitting nicely with the instrumentation chapter is a series of articles on ion mobilities (Chapter 7). These three articles give a picture of the theory of ion mobilities and how they can be applied to the applications of structure elucidation.

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The two yet-to-be-mentioned chapters (Chapter 12, “Inorganic Chemistry,” and Chapter 13, “Biopolymers”) are both important and bracket the breath of the technology covered in this book. The five articles in the inorganic chapter cover some of the more obscure areas of inorganic mass spectrometry theory that are often ignored, but provide a wealth of information about gas-phase ion behavior. Two of the articles in the biopolymer section, “H/D Exchange Reactions of Biological Molecules in the Gas Phase” and “Ion–Ion Reactions,” provide an understanding of some of the phenomena that allow for the understanding of the behavior of large ions that are now becoming ubiquitous in mass spectrometry.

In the Volume Preface, Peter Armentrout acknowledges that the volume is not as complete as he desired due to problems in getting articles from some who committed but, in the end, did not fulfill their commitment. Having undertaken a similar endeavor, I am quite aware of these difficulties. Also in the Preface, Armentrout expresses appreciation to the authors of the various articles for tolerating his “editorial preferences.” This insistence on these preferences and Armentrout’s careful editing is evident in the consistent style that is throughout all the articles. Although not a requirement of the editors-in-chief or the publisher, the volume editor did use the review process for various articles to assure the highest quality and the most accurate information. As this volume is used by a researcher, the added burden of switching styles and nomenclature will be avoided as the sometimes very esoteric topics are detailed. Although not listed in the usual fashion, Armentrout points out in the Preface the editorial board who helped shape this volume: Tom Bear, Jack Beauchamp, and Veronica Bierbaum. Such a quartet could only assemble as comprehensive a collection of topics as this volume.

Of the over 3,900 citations in the book, only a handful of the cited journal articles (probably less than 10) do not have the article’s title. This is probably a first for a book on the fundamentals of mass spectrometry. The book is filled with high-quality illustrations that have clear legends, which adds to the clarity of the text. Many of these illustrations are original rather than recycling material that has been seen many times before. The articles have section headings that make for ease of jumping around for overview purposes or reclassification of specific areas. The two-column format with a head-to-tail style for the articles makes for easy reading.

The only real shortcoming I found for this volume was a lack of “suggested further reading” references. The only article to include such a listing was the “TOF and RTOF” article in Chapter 3, “Instrumentation.” Many encyclopedic articles are written totally without references with only a list of “suggested further readings” at the end. I prefer the use of citations to support the various aspects of the article as is done with this book; but feel that to serve as a true reference, the user

should be provided with other, perhaps more detailed, seminal sources.

One other possible shortcoming of this volume is the lack of an introductory article or preface for each chapter. Unlike most encyclopedias, this book does not have the articles arranged in alphabetical order by subject. The articles are logically grouped into chapters. However, each chapter begins with the first article in that chapter without any explanation of the chapter. An article that tied the articles in the chapter together would have been nice; but, on the other hand, that would make this more like a reference or text book and less like an encyclopedia.

Because my current interest is in the teaching of mass spectrometry, I have emphasized these aspects of the outstanding volume. However, this book will also have appeal to and be used by practitioners, who far outnumber those who will employ it as a teaching aid, wanting to understand ion chemistry, instrument design, and the overall functions of mass spectrometry. This collection of articles will be timeless. It will save countless hours of searching through many references to accumulate the knowledge that is contained in this comprehensive volume. Even before I completed this review, I found material that I used in the course that I taught in the Fall of 2003. This book has made my preparations much easier and allowed my students to spend more time in learning and less time digging through the literature. The production quality is the highest that I have seen in a long time. This is very important due to the heavy handling by numerous students and researchers who will be using this book over the years. And it will be in use for many years for other than just historical reference because much of the information involves well-defined physics that will not change. One final comment is with regard to the price of this volume. I am often very critical of the price of books today; however, at an average price of \$4.95 per article, *The Encyclopedia of Mass Spectrometry, Volume 1: Theory and Ion Chemistry*, Peter B. Armentrout, Editor, is an excellent value. This book will serve research libraries for many years to come and will provide a foundation for the learning of mass spectrometry theory and ion chemistry for countless students. This book will also make a proper parting gift for the students who have distinguished themselves in university laboratories dedicated to the study of the chemistry and physics of mass spectrometry.

List of Articles appearing in *The Encyclopedia of Mass Spectrometry, Volume 1: Theory and Ion Chemistry*:

#### Chapter 1: Theory (Reactions)

##### Ion-Molecule Collision Theory

D. P. Ridge (University of Delaware, Newark, Delaware, USA)

##### Statistical Theories in Mass Spectrometry

J. C. Lorquet (Université de Liège, Belgium)

B. Leyh (Université de Liège, Belgium)

Kinetic Energy Release Distributions in Mass Spectrometry

B. Leyh (Université de Liège, Belgium)

J. C. Lorquet (Université de Liège, Belgium)

Non-adiabatic Reactions

J. C. Lorquet (Université de Liège, Belgium)

B. Leyh (Université de Liège, Belgium)

Classical Trajectory Simulations

W. L. Hase (Wayne State University, Detroit, Michigan, USA)

Chapter 2: Theory (Energies and Potential Energy Surfaces)

Theoretical Methods

M. S. Gordon (Iowa State University, Ames, Iowa, USA)

Anions

J. Simons (University of Utah, Salt Lake City, Utah, USA)

Organics

M. Yáñez (Universidad Autónoma de Madrid, Spain)

Transition Metals

M. C. Holthausen (Phillips-Universität Marburg, Germany)

Chapter 3: Instrumentation

Metastable Ions

J. L. Holmes (University of Ottawa, Ontario, Canada)

Flow Tubes

V. M. Bierbaum (University of Colorado, Boulder, Colorado, USA)

Multiquadrupoles

C. Rolando (Université des Sciences et Technologies de Lille, Villeneuve d'Ascq, France)

M. Sablier (Ecole Polytechnique, Palaiseau, France)

TOF and RTOF

A. Uphoff (Christian Albrechts Universität zu Kiel, Germany)

J. Grotemeyer (Christian Albrechts Universität zu Kiel, Germany)

Fourier Transform Ion Cyclotron Resonance

A. G. Marshall (Florida State University, Tallahassee, Florida, USA)

Ion Traps

R. E. March (Trent University, Peterborough, Ontario, Canada)

Crossed Beam Methods for Ion Collisions

J. M. Farrar (University of Rochester, New York, USA)

Merged Beams

W. R. Gentry (University of Minnesota, Minneapolis, Minnesota, USA)

RF Ion Guides

D. Gerlich (Technische Universität, Chemnitz, Germany)

Ion Storage Rings

M. Larsson (Stockholm University, Sweden)

High-temperature Studies

A. A. Viggiano (Air Force Research Laboratory, Hanscom AFB, Massachusetts, USA)

Chapter 4: Ion Spectroscopy

Spectroscopy of Molecular Ions in Noble Gas Matrices

L. Andrews (University of Virginia, Charlottesville, Virginia, USA)

Microwave and Infrared Spectroscopy of Molecular Ions

T. Oka (University of Chicago, Illinois, USA)

Ion Fluorescence

T. G. Wright (University of Sussex, Brighton, UK)

Photoelectron Spectroscopy, Threshold Photoelectron Spectroscopy, and Pulsed Field Ionization

T. Baer (University of North Carolina, Chapel Hill, North Carolina, USA)

Threshold Ion-pair Production Spectroscopy (TIPPS)

J. W. Hepburn (University of British Columbia, Vancouver, British Columbia, Canada)

Photodissociation Spectroscopy

R. C. Dunbar (Case Western Reserve University, Cleveland, Ohio, USA)

Infrared Photodissociation

J. M. Riveros (Universidade de São Paulo, Brazil)

Vibrational Predissociation

M. A. Johnson (Yale University, New Haven, Connecticut, USA)

Product State Distributions

S. Kato (University of Colorado, Boulder, Colorado, USA)

Vibrational State Selection

S. L. Anderson (University of Utah, Salt Lake City, Utah, USA)

Ion Imaging Techniques for the Measurement of Ion Velocities

D. W. Chandler (Sandia National Laboratory, Livermore, California, USA)

C. C. Hayden (Sandia National Laboratory, Livermore, California, USA)

#### Chapter 5: Thermochemistry (Methods)

##### Thermochemistry Definitions and Tabulations

K. M. Ervin (University of Nevada, Reno, Nevada, USA)

P. B. Armentrout (University of Utah, Salt Lake City, Utah, USA)

##### The Bracketing Method for Determining the Thermochemistry of Ion–Molecule Reactions

J. E. Bartmess (University of Tennessee, Knoxville, Tennessee, USA)

##### Ion–Molecule Equilibria at High Pressure

P. Kebarle (University of Alberta, Edmonton, Alberta, Canada)

##### Low-pressure Ion–Molecule Equilibrium

K. A. Kellersberger (Brigham Young University, Provo, Utah, USA)

D. V. Dearden (Brigham Young University, Provo, Utah, USA)

##### Charge Transfer Equilibria and Complexes

M. Meot-Ner (Mautner) (University of Canterbury, Christchurch, New Zealand)

##### The Kinetic Method: Thermochemical Determinations and Chiral Analysis

X. Zheng (Purdue University, West Lafayette, Indiana, USA)

R. Augusti (Universidade Federal de Minas Gerais, Belo Horizonte, Brazil)

W. A. Tao (The Institute for Systems Biology, Seattle, Washington, USA)

R. G. Cooks (Purdue University, West Lafayette, Indiana, USA)

##### Radiative Association Kinetics: Ion–Ligand Binding Thermochemistry

R. C. Dunbar (Case Western Reserve University, Cleveland, Ohio, USA)

##### Black-body Infrared Radiative Dissociation (BIRD)

R. C. Dunbar (Case Western Reserve University, Cleveland, Ohio, USA)

##### Measuring Fragment Ion Appearance Energies by Photoionization Methods

T. Baer (University of North Carolina, Chapel Hill, North Carolina, USA)

##### Photoelectron Spectroscopy of Negative Ion Beams: Measurements of Electron Affinities

G. B. Ellison (University of Colorado, Boulder, Colorado, USA)

##### Thermochemistry from Threshold Ion-pair Production Spectroscopy

J. W. Hepburn (University of British Columbia, Vancouver, British Columbia, Canada)

##### Photodissociation Studies of Ion Thermochemistry

R. C. Dunbar (Case Western Reserve University, Cleveland, Ohio, USA)

##### Reaction Threshold Energy Measurements

P. B. Armentrout (University of Utah, Salt Lake City, Utah, USA)

##### Collision-induced Dissociation

P. B. Armentrout (University of Utah, Salt Lake City, Utah, USA)

##### The Correlation of Thermochemical Data

J. L. Holmes (University of Ottawa, Ontario, Canada)

#### Chapter 6: Collisional Activation and Dissociation

##### Methodology

J. M. Wells (Purdue University, West Lafayette, Indiana, USA)

S. A. McLuckey (Purdue University, West Lafayette, Indiana, USA)

##### Single Collisions

P. B. Armentrout (University of Utah, Salt Lake City, Utah, USA)

##### Multiply Charged Ions

P. Scheier (Institut für Ionenphysik, Innsbruck, Austria)

##### Collisional Activation for Structural Analysis

D. Schröder (Technische Universität Berlin, Germany)

##### Via Ion–Neutral Complexes

T. H. Morton (University of California, Riverside, California, USA)

##### Collisions of Ions with Surfaces at Hyperthermal Energies

R. G. Cooks (Purdue University, West Lafayette, Indiana, USA)

V. Grill (Purdue University, West Lafayette, Indiana, USA)

N. Wade (Purdue University, West Lafayette, Indiana, USA)

S.-C. Jo (Purdue University, West Lafayette, Indiana, USA)

B. Gologan (Purdue University, West Lafayette, Indiana, USA)

#### Chapter 7: Mobilities

##### Transport Properties

L. A. Viehland (Chatham College, Pittsburgh, Pennsylvania, USA)

##### Small Systems

J. Husband (University of Colorado, Boulder, Colorado, USA)

S. R. Leone (University of Colorado, Boulder, Colorado, USA)

##### Drift Tubes: Instrumentation and Applications to Biomolecules

A. E. Hilderbrand (Indiana University, Bloomington, Indiana, USA)

S. J. Valentine (Beyond Genomics, Inc., Waltham, Massachusetts, USA)

D. E. Clemmer (Indiana University, Bloomington, Indiana, USA)

#### Chapter 8: Neutralization, Charge Reversal

##### Charge Reversal

D. Schröder (Technische Universität Berlin, Germany)

##### Generation and Characterization of Transient Intermediates by —Neutralization—Reionization Mass Spectrometry

F. Tureček (University of Washington, Seattle, Washington, USA)

##### Electron–Ion Recombination

N. G. Adams (University of Georgia, Athens, Georgia, USA)

L. M. Babcock (University of Georgia, Athens, Georgia, USA)

J. L. McLain (University of Georgia, Athens, Georgia, USA)

##### Ion–Ion Recombination

N. G. Adams (University of Georgia, Athens, Georgia, USA)

L. M. Babcock (University of Georgia, Athens, Georgia, USA)

C. D. Molek (University of Georgia, Athens, Georgia, USA)

#### Chapter 9: Organic Ion Chemistry (Positive)

##### Unimolecular Organic Reactions

N. M. M. Nibbering (Vrije Universiteit, Amsterdam, The Netherlands, and University of Twente, Enschede, The Netherlands)

##### Bimolecular Reactions

N. M. M. Nibbering (Vrije Universiteit, Amsterdam, The Netherlands, and University of Twente, Enschede, The Netherlands)

##### Aliphatic Substitution

D. Kuck (Universität Bielefeld, Germany)

##### Electrophilic Aromatic Substitution

D. Kuck (Universität Bielefeld, Germany)

##### S<sub>N</sub>2 and Related Reactions

R. A. J. O'Hair (University of Melbourne, Victoria, Australia)

##### Distonic Radical Cations

H. I. Kenttämaa (Purdue University, West Lafayette, Indiana, USA)

##### Gas-phase H/D Exchange of Organic Compounds for Structural Elucidation

M. K. Green (McMaster University, Hamilton, Canada)

C. B. Lebrilla (University of California, Davis, California, USA)

#### Chapter 10: Organic Ion Chemistry (Negative)

##### Unimolecular Rearrangements of Carbanions

S. R. Kass (University of Minnesota, Minneapolis, Minnesota, USA)

##### Nucleophilic Substitution and Elimination Reactions

S. Gronert (San Francisco State University, California, USA)

##### Addition/Elimination Reactions

S. Gronert (San Francisco State University, California, USA)

##### Oxidation/Reduction Reactions of Negative Ions in the Gas Phase

P. G. Wenthold (Purdue University, West Lafayette, Indiana, USA)

##### Strained Ring and Highly Basic Carbanions

S. R. Kass (University of Minnesota, Minneapolis, Minnesota, USA)

##### Negative Distonic Ions

N. M. M. Nibbering (Vrije Universiteit, Amsterdam, The Netherlands, and University of Twente, Enschede, The Netherlands)

##### H/D Exchange Reactions

C. H. DePuy (University of Colorado, Boulder, Colorado, USA)

S. Kato (University of Colorado, Boulder, Colorado, USA)

##### Organoaluminum, -silicon, -phosphorus, and -sulfur Chemistry

R. Damrauer (University of Colorado at Denver, Colorado, USA)

R. A. J. O'Hair (University of Melbourne, Victoria, Australia)

#### Chapter 11: Solvation and Clusters

##### The Ionic Hydrogen Bond: Clusters and Ion Solvation

M. Meot-Ner (Mautner) (University of Canterbury, Christchurch, New Zealand)

##### Charge Transfer Complexes

M. Meot-Ner (Mautner) (University of Canterbury, Christchurch, New Zealand)

##### Small Molecular Clusters

R. L. DeLeon (The State University of New York, Buffalo, New York, USA)

J. F. Garvey (The State University of New York, Buffalo, New York, USA)

##### Covalent Clusters of Group 14 Elements

C. Lifshitz (The Hebrew University of Jerusalem, Israel)

### Endohedral Complexes of Fullerenes and Mass Spectrometry

D. E. Giblin (Washington University, St. Louis, Missouri, USA)

M. L. Gross (Washington University, St. Louis, Missouri, USA)

### Cluster Anions (Experiments)

K. H. Bowen, Jr. (Johns Hopkins University, Baltimore, Maryland, USA)

E. W. Schlag (Technische Universität Munich, Garching, Germany)

### Metal Ion Solvation

P. B. Armentrout (University of Utah, Salt Lake City, Utah, USA)

### Host–Guest Chemistry in the Gas Phase

D. V. Dearden (Brigham Young University, Provo, Utah, USA)

### Metal Clusters

K. Hansen (Gothenburg University and Chalmers University of Technology, Gothenburg, Sweden)

L. Schweikhard (Ernst-Moritz-Arndt-Universität, Greifswald, Germany)

## Chapter 12: Inorganic Chemistry

### Alkali Metal Ion Chemistry

J. D. Anderson (Brigham Young University, Provo, Utah, USA)

D. V. Dearden (Brigham Young University, Provo, Utah, USA)

### Silicon Ion Chemistry

D. K. Bohme (York University, Toronto, Ontario, Canada)

### Transition Metal Ion Chemistry

P. B. Armentrout (University of Utah, Salt Lake City, Utah, USA)

### Transition Metal Oxides

D. Schröder (Technische Universität Berlin, Germany)

### Photoelectron Spectroscopy of Inorganic Molecules

N. E. Gruhn (University of Arizona, Tucson, Arizona, USA)

D. L. Lichtenberger (University of Arizona, Tucson, Arizona, USA)

## Chapter 13: Biopolymers

### The Ionic Hydrogen Bond in Complex Organics and Biomolecules

M. Meot-Ner (Mautner) (University of Canterbury, Christchurch, New Zealand)

### H/D Exchange Reactions of Biological Molecules in the Gas Phase

J. L. Beauchamp (California Institute of Technology, Pasadena, California, USA)

### Ion–Ion Reactions

S. A. McLuckey (Purdue University, West Lafayette, Indiana, USA)

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remote/dit/data/elsevier/pdf/0f1/aHR0cDovL2FwaS5lbHNldmllci5jb20vY29udGVudC9hcnRpY2xlL3BpaS9zMTA0NDZMDUwNDAwMTc4Mw==.pdf.

Suggested articles. Editors: Michael L. Gross Richard Caprioli. Hardcover ISBN: 9780080438016. Imprint: Elsevier Science.Â Volume 6: Ionization Methods captures the story of molecular ionization and its phenomenal evolution that makes mass spectrometry the powerful method it is today. Chapters 1 and 2 cover fundamentals and various issues that are common to all ionization (e.g., accurate mass, isotope clusters, and derivatization). Chapters 3-9 acknowledge that some ionization methods are appropriate for gas-phase molecules and others for molecules that are in the solid or liquid states.Â Electrospray and MALDI also lead to applications in biophysical chemistry, the theme of Chapter 10. Chapter 11 reconsiders ionization from the view of choosing an ionization method. This volume is the first in the multi-volume work, providing unparalleled and comprehensive coverage of the full range of topics and techniques Suitable for new graduate students who are interested but not yet versed in the subject of mass spectrometry Techniques, methods and applications of mass spectrometry are described in considerable detail; including limitations, current problems, and areas in which the method does not succeed well.Â Theory and Ion Chemistry concentrates on the fundamental aspects of a set of 13 carefully chosen topics covering the whole field of mass spectrometry.