
Mass Spectrometry

Jürgen H. Gross

Mass Spectrometry

A Textbook

Third Edition

 Springer

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Preface

When non-mass spectrometrists are talking about mass spectrometry, it rather often sounds as if they were telling a story out of Poe's *Tales of Mystery and Imagination*. Indeed, mass spectrometry appears to be regarded as a mysterious method, just good enough to supply some molecular weight information. Unfortunately, this rumor about the dark side of analytical methods may reach students way before their first contact with mass spectrometry. Possibly, some of this may have been bred by some mass spectrometrists who used to celebrate each mass spectrum they obtained from the very first gigantic machines of the early days. Of course, there were also those who enthusiastically started in the 1950s toward developing mass spectrometry out of the domain of physics to become a new analytical tool for chemistry. Within the more than a hundred years since J. J. Thomson's seminal work, there has been a lot that has happened and a lot now to be known and learned about mass spectrometry.

How All This Began

Back in the late 1980s, J. J. Veith's mass spectrometry laboratory at the Technical University of Darmstadt was bright and clean, had no noxious odors, and thus presented a nice contrast to a preparative organic chemistry laboratory. Numerous stainless steel flanges and electronics cabinets were tempting to be explored and – whoops – infected me with CMSD (chronic mass spectrometry disease). Staying with Veith's group slowly transformed me into a mass spectrometrist. Inspiring books such as *Fundamental Aspects of Organic Mass Spectrometry* or *Metastable Ions*, out of stock even in those days, did help me very much during my metamorphosis. Having completed my doctoral thesis on fragmentation pathways of isolated immonium ions in the gas phase, I assumed my current position. Since 1994, I have been head of the mass spectrometry laboratory at the Chemistry Department of Heidelberg University where I teach introductory courses and seminars on mass spectrometry.

When students then asked what books to read on mass spectrometry, there were various excellent monographs, but the ideal textbook still seemed to be missing – at least in my opinion. Finally, 2 years of writing began.

A Third Edition

Now, *Mass Spectrometry – A Textbook* is here in its third edition. For me, the author, preparing the third edition meant an obligation to update and further improve the content of this book. The extent of overall coverage and global organization has not changed as much for this edition as in the transition from the first to the second edition – nonetheless, many new sections have been added to adequately present the recent innovations in this ever-developing field of mass spectrometry. No chapter has remained untouched. Each of the 15 chapters has carefully been reworked and augmented with hundreds of additions, changes, and corrections.

What's New?

Since the second edition, new techniques have gained importance, and some instrumentation has received notable attention and attained considerable commercial success. To keep pace with recent developments, Chap. 4 now includes TOF instruments with folded flight paths, the dynamically harmonized FT-ICR cell, more on hybrid instruments, and ion mobility spectrometry–mass spectrometry. The increasing relevance of high-resolution and accurate mass measurements is even strongly reflected in Chap. 3. The five chapters dedicated to soft ionization methods (CI, APCI, APPI, FAB, LSIMS, FI, FD, LIFDI, ESI, LDI, MALDI) as well as those on ambient desorption/ionization (DESI, DART, REIMS, etc.) and on tandem mass spectrometry have been substantially updated and upgraded. There is also much more on chromatographic techniques (GC, LC) and their coupling to mass spectrometry in Chap. 14.

The way we are using books and literature in general has dramatically changed during the last decade. Back in 2001, when I started preparing the first edition of this book, regular visits to the libraries of several institutions in the area were on my schedule to collect some vast amount of literature. Today, almost all journal articles are electronically available within seconds, and even textbooks are now being extensively used in their e-book versions. This had also some impact on the layout and production process of this book.

In the light of an ever-growing abundance of methods, instruments, tools, and rules in mass spectrometry, the ease of how a complex field of analytical science can be grasped mentally certainly deserves attention. Therefore, the emphasis of my work was on refinement in terms of presentation, convenience of use, and ease of learning. Obviously, a textbook ranging around 900 pages may deter the novice, and thus, my focus was on a didactic and educational approach. Although the actual number of pages has notably increased once again, you will find the textbook easier to read, and you will benefit when transferring theory in actual practice such as spectral interpretation and method selection.

Overall, the third edition of *Mass Spectrometry – A Textbook* comes with lots of didactical improvements:

- Numerous passages have been rewritten and improved while remaining short and concise. Care has been taken not only to explain *how* but also *why* things are done a particular way.
- The number of figures has been notably increased, and about one third of them are now in full color. More photographs and schematics mean easier comprehension of contents, often providing valuable insight into the practical aspects of instrumentation and according procedures.
- Flowcharts have been introduced to describe procedures and approaches to mass spectral interpretation or aid in decision making.
- Bulleted enumerations have been introduced wherever a larger number of features, arguments, assumptions, or properties regarding a subject warrant a clear presentation.
- More examples, especially of methods and applications, are given and some *how-to-style* paragraphs provide practical guidance.
- Examples and notes now come with a short subheading that immediately tells what the particular section is all about.
- All chapters conclude with a concise summary that is subdivided into compact sections highlighting the basic concepts of the subject area, its figures of merit, typical applications, and its role in current MS. Chapter 4 (“Instrumentation”) provides summaries of all types of mass analyzers.
- Digital object identifiers (DOIs) are included in the lists of references to facilitate the retrieval of references for e-book users. For those of you who, like me, still prefer a hardbound book, the DOIs offer an additional level of comfort. So, I am pretty convinced that the tedious work of collecting DOIs was very much worth the effort.
- The book’s website has been updated providing new exercises and supplementary material (www.ms-textbook.com).

Deepest Gratitude

To all readers of the previous editions of *Mass Spectrometry – A Textbook*, I would like to express my deepest gratitude. Without their interest in wanting to learn more about mass spectrometry by the use of this book, all the efforts in writing it would have been a mere waste of time, and moreover, without their demand for updates, there would be no next edition. I also would like to thank the instructors all over the world who adopted and recommended this book for their own mass spectrometry courses.

Being an author of a textbook means to retrieve, collect, compile, sort, and balance knowledge, findings, and inventions of others. Most of what is written here relies on the intelligence, skill, integrity, and devotion of hundreds of researchers who have contributed to mass spectrometry each in their own way.

Many kind people have supported me in the process of compiling this and the previous editions. I appreciate the detailed knowledge and great thoroughness allocated by Kenzo Hiraoka, Yasuhide Naito, Takemichi Nakamura, and Hiroaki Sato to the translation of the first edition into Japanese. The valuable and welcome comments from readers from all over the world and, in particular, from book reviewers and colleagues have revealed some shortcomings, which now could be adequately addressed.

For the second edition, several competent and renowned colleagues had contributed by carefully checking the according contents in their fields of expertise. I want to express my special thanks to Jürgen Grotemeyer, University of Kiel, for checking Chap. 2 (“Principles of Ionization and Ion Dissociation”); Alexander Makarov, Thermo Fisher Scientific, Bremen (Chap. 4, “Instrumentation”); Christoph A. Schalley, Freie Universität Berlin (Chap. 9, “Tandem Mass Spectrometry”); Belá Paizs, German Cancer Research Center, Heidelberg (Chap. 11, “Matrix-Assisted Laser Desorption/Ionization”); Zoltán Takáts, Universität Gießen (Chap. 13, “Ambient Mass Spectrometry”); and Detlef Günther, ETH Zürich (Chap. 15, “Inorganic Mass Spectrometry”).

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Again, many manufacturers of mass spectrometers and mass spectrometry supply are gratefully acknowledged for generously providing schemes and photographs. The author wishes to express his thanks to those scientists, many of them from Heidelberg University, who allowed to use material from their research as examples and to those publishers, who granted the numerous copyrights for the use of figures from their publications. The generous permission of the National Institute of Standards and Technology (S. Stein, G. Mallard, J. Sauerwein) to use a large set of electron ionization mass spectra from the NIST/EPA/NIH Mass Spectral Library is also gratefully acknowledged.

Permission to prepare this third edition alongside my official professional duties, granted by Oliver Trapp, former director of OCI, and Heinfried Schöler, former dean of the Faculty of Chemistry and Earth Sciences, is sincerely acknowledged. Many thanks to my team Doris Lang, Iris Mitsch, and Norbert Nieth for smoothly running the routine analyses in our MS facility. Once more, Theodor C. H. Cole accomplished a great job in polishing up my English. Finally, I am again grateful to my family for their patience and solidarity in times when I had to come home late or needed to vanish on Saturdays during the writing of this book.

Have a good time studying, learning, and enjoying the world of mass spectrometry!

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Contents

1	Introduction	1
1.1	Mass Spectrometry: Versatile and Indispensable	1
1.2	Historical Sketch	3
1.2.1	The First Mass Spectra	3
1.2.2	Thomson's Parabola Spectrograph	3
1.2.3	Milestones	4
1.3	Aims and Scope of This Textbook	5
1.3.1	Facets of Mass Spectrometry	7
1.4	What Is Mass Spectrometry?	7
1.4.1	Basic Principle of Mass Spectrometry	8
1.4.2	Mass Spectrometer	9
1.4.3	Mass Scale	10
1.4.4	Mass Spectrum	11
1.4.5	Statistical Nature of Mass Spectra	12
1.4.6	Bars, Profiles, and Lists	14
1.5	Ion Chromatograms	14
1.6	Performance of Mass Spectrometers	17
1.6.1	Sensitivity	17
1.6.2	Limit of Detection	18
1.6.3	Signal-to-Noise Ratio	18
1.7	Terminology – General Aspects	19
1.7.1	Basic Terminology in Describing Mass Spectra	20
1.8	Units, Physical Quantities, and Physical Constants	21
1.9	Further Reading	21
1.10	Quintessence	22
	References	22
2	Principles of Ionization and Ion Dissociation	29
2.1	Gas Phase Ionization by Energetic Electrons	30
2.1.1	Formation of Ions	30
2.1.2	Processes Accompanying Electron Ionization	31
2.1.3	Ions Generated by Penning Ionization	32

2.1.4	Ionization Energy	34
2.1.5	Ionization Energy and Charge-Localization	34
2.2	Vertical Transitions	36
2.3	Ionization Efficiency and Ionization Cross Section	38
2.4	Internal Energy and the Further Fate of Ions	40
2.4.1	Degrees of Freedom	40
2.4.2	Appearance Energy	41
2.4.3	Bond Dissociation Energies and Heats of Formation	42
2.4.4	Randomization of Energy	45
2.5	Quasi-Equilibrium Theory	47
2.5.1	QET's Basic Premises	48
2.5.2	Basic QET	48
2.5.3	Rate Constants and Their Meaning	50
2.5.4	$k_{(E)}$ Functions – Typical Examples	50
2.5.5	Reacting Ions Described by $k_{(E)}$ Functions	51
2.5.6	Direct Cleavages and Rearrangement Fragmentations	51
2.6	Time Scale of Events	52
2.6.1	Stable, Metastable, and Unstable Ions	53
2.6.2	Time Scale of Ion Storage Devices	55
2.7	Internal Energy – Practical Implications	56
2.8	Reverse Reactions – Activation Energy and Kinetic Energy Release	57
2.8.1	Activation Energy of the Reverse Reaction	57
2.8.2	Kinetic Energy Release	58
2.8.3	Energy Partitioning	59
2.9	Isotope Effects	60
2.9.1	Primary Kinetic Isotope Effects	60
2.9.2	Measurement of Isotope Effects	62
2.9.3	Secondary Kinetic Isotope Effects	64
2.10	Determination of Ionization Energies	65
2.10.1	Conventional Determination of Ionization Energies	65
2.10.2	Improved <i>IE</i> Accuracy from Data Post-processing	65
2.10.3	<i>IE</i> Accuracy – Experimental Improvements	66
2.10.4	Photoionization Processes	66
2.10.5	Photoelectron Spectroscopy and Derived Methods	68
2.10.6	Mass-Analyzed Threshold Ionization	68
2.11	Determining the Appearance Energies	70
2.11.1	Kinetic Shift	70
2.11.2	Breakdown Graphs	71
2.12	Gas Phase Basicity and Proton Affinity	73
2.13	Ion–Molecule Reactions	74
2.13.1	Reaction Order	75
2.13.2	Solution Phase Versus Gas Phase Reactions	76

2.14	Summary of Gas Phase Ion Chemistry	78
	References	79
3	Isotopic Composition and Accurate Mass	85
3.1	Isotopic Classification of the Elements	86
3.1.1	Monoisotopic Elements	86
3.1.2	Di-isotopic Elements	86
3.1.3	Polyisotopic Elements	87
3.1.4	Representation of Isotopic Abundances	87
3.1.5	Calculation of Atomic, Molecular, and Ionic Mass	88
3.1.6	Natural Variations in Relative Atomic Mass	93
3.2	Calculation of Isotopic Distributions	95
3.2.1	Carbon: An X + 1 Element	95
3.2.2	Terms Related to Isotopic Composition	97
3.2.3	Binomial Approach	98
3.2.4	Halogens	98
3.2.5	Combinations of Carbon and Halogens	101
3.2.6	Polynomial Approach	102
3.2.7	Oxygen, Silicon, and Sulfur	104
3.2.8	Polyisotopic Elements	106
3.2.9	Practical Aspects of Isotopic Patterns	106
3.2.10	Bookkeeping with Isotopic Patterns in Mass Spectra	108
3.2.11	Information from Complex Isotopic Patterns	109
3.2.12	Systematic Approach to Reading Isotopic Patterns	109
3.3	Isotopic Enrichment and Isotopic Labeling	110
3.3.1	Isotopic Enrichment	110
3.3.2	Isotopic Labeling	112
3.4	Resolution and Resolving Power	112
3.4.1	Definitions	112
3.4.2	Resolution and Its Experimental Determination	113
3.4.3	Resolving Power and Its Effect on Relative Peak Intensity	114
3.5	Accurate Mass	115
3.5.1	Exact Mass and Molecular Formulas	116
3.5.2	Relativistic Mass Defect	117
3.5.3	Role of Mass Defect in Mass Spectrometry	117
3.5.4	Mass Accuracy	119
3.5.5	Accuracy and Precision	120
3.5.6	Mass Accuracy and the Determination of Molecular Formulas	121
3.5.7	Extreme Mass Accuracy: Special Considerations	122
3.6	Applied High-Resolution Mass Spectrometry	123
3.6.1	Mass Calibration	123
3.6.2	Performing an External Mass Calibration	124
3.6.3	Internal Mass Calibration	128

3.6.4	Specification of Mass Accuracy	129
3.6.5	Identification of Formulas from HR-MS Data	131
3.7	Resolution Interacting with Isotopic Patterns	132
3.7.1	Multiple Isotopic Compositions at Very High Resolution	132
3.7.2	Isotopologs and Accurate Mass	135
3.7.3	Large Molecules – Isotopic Patterns at Sufficient Resolution	137
3.7.4	Isotopic Patterns of Macromolecules Versus Resolution	139
3.8	Charge State and Interaction with Isotopic Patterns	140
3.9	Approaches to Visualize Complex HR-MS Data Sets	142
3.9.1	Deltamass	142
3.9.2	Kendrick Mass Scale	143
3.9.3	Van Krevelen Diagrams	144
3.10	Vantage Point on the World of Isotopes and Masses	145
	References	146
4	Instrumentation	151
4.1	How to Create a Beam of Ions	154
4.2	Time-of-Flight Instruments	155
4.2.1	Time-of-Flight: Basic Principles	155
4.2.2	TOF Instruments: Velocity of Ions and Time-of-Flight	157
4.2.3	Linear Time-of-Flight Analyzer	159
4.2.4	Better Vacuum Improves Resolving Power	161
4.2.5	Energy Spread of Laser-Desorbed Ions	161
4.2.6	Reflector Time-of-Flight Analyzer	163
4.2.7	Delay Before Extraction to Improve Resolving Power	165
4.2.8	Orthogonal Acceleration TOF Analyzers	167
4.2.9	Operation of the oaTOF Analyzer	169
4.2.10	Duty Cycle	170
4.2.11	TOF Analyzers with a Folded Eight-Shaped Flight Path	171
4.2.12	Multi-reflecting TOFs	174
4.2.13	Essence of TOF Instruments	176
4.3	Magnetic Sector Instruments	177
4.3.1	Evolution of Magnetic Sector Instruments	177
4.3.2	Principle of the Magnetic Sector	178
4.3.3	Focusing Action of the Magnetic Field	180
4.3.4	Double-Focusing Sector Instruments	181
4.3.5	Geometries of Double-Focusing Sector Instruments	183
4.3.6	Adjusting the Resolving Power of a Sector Instrument	186

4.3.7	Optimization of Sector Instruments	186
4.3.8	Summary of Magnetic Sector Instruments	189
4.4	Linear Quadrupole Instruments	190
4.4.1	Introduction	190
4.4.2	The Linear Quadrupole	190
4.4.3	Resolving Power of Linear Quadrupoles	196
4.4.4	RF-Only Quadrupoles, Hexapoles, and Octopoles	197
4.5	Linear Quadrupole Ion Traps	201
4.5.1	Linear RF-Only Multipole Ion Traps	201
4.5.2	Mass-Analyzing Linear Quadrupole Ion Trap with Axial Ejection	203
4.5.3	Mass-Analyzing Linear Ion Trap with Radial Ejection	207
4.5.4	Constructing an Instrument Around the LIT	208
4.6	Ion Trap with Three-Dimensional Quadrupole Field	210
4.6.1	Introduction	210
4.6.2	Principle of the Quadrupole Ion Trap	211
4.6.3	Visualization of Ion Motion in the Ion Trap	214
4.6.4	Mass-Selective Stability Mode	214
4.6.5	Mass-Selective Instability Mode	215
4.6.6	Resonant Ejection	215
4.6.7	Axial Modulation and Control of the Ion Population	216
4.6.8	Nonlinear Resonances	217
4.6.9	Miniaturization and Simplification of Ion Traps	219
4.6.10	Digital Waveform Quadrupole Ion Trap	221
4.6.11	External Ion Sources for the Quadrupole Ion Trap	222
4.6.12	Ion Trap Maintenance	223
4.6.13	Summary of RF Quadrupole Devices	224
4.7	Fourier Transform Ion Cyclotron Resonance	225
4.7.1	From Ion Cyclotron Resonance to Mass Spectrometry	225
4.7.2	Ion Cyclotron Motion – Basics	226
4.7.3	Cyclotron Motion: Excitation and Detection	227
4.7.4	Cyclotron Frequency Bandwidth and Energy-Time Uncertainty	230
4.7.5	Fourier Transform – Basic Properties	232
4.7.6	Nyquist Criterion	234
4.7.7	Excitation Modes in FT-ICR-MS	235
4.7.8	Axial Trapping	237
4.7.9	Magnetron Motion and Reduced Cyclotron Frequency	237
4.7.10	Detection and Accuracy in FT-ICR-MS	238
4.7.11	Design of ICR Cells	241
4.7.12	FT-ICR Instruments	243
4.7.13	Summary of FT-ICR Instrumentation	245

4.8	Orbitrap Analyzer	246
4.8.1	Orbitrap – Principle of Operation	247
4.8.2	Ion Detection and Resolving Power of the Orbitrap	249
4.8.3	Ion Injection into the Orbitrap	249
4.8.4	Hybridization with a Linear Quadrupole Ion Trap	252
4.8.5	Orbitrap at a Glance	253
4.9	Hybrid Instruments	254
4.9.1	Evolution of Hybrid Mass Spectrometers	255
4.10	Ion Mobility-Mass Spectrometry Systems	257
4.10.1	Ion Mobility Separation	259
4.10.2	Stacked Ring Ion Guide	260
4.10.3	Traveling Wave Ion Guides for IMS	262
4.10.4	Hybrid Instruments with IMS	264
4.10.5	Overview of Hybrid Instrumentation Including IM-MS	265
4.11	Ion Detection	266
4.11.1	Analog-to-Digital Conversion	266
4.11.2	Digitization Rate	267
4.11.3	Time-to-Digital Conversion	267
4.11.4	Discrete Dynode Electron Multipliers	268
4.11.5	Channel Electron Multipliers	269
4.11.6	Microchannel Plates	270
4.11.7	Post-acceleration and Conversion Dynode	271
4.11.8	Focal Plane Detectors	272
4.12	Vacuum Technology	273
4.12.1	Basic Mass Spectrometer Vacuum System	273
4.12.2	High Vacuum Pumps	274
4.13	Purchasing an Instrument	275
	References	277
5	Practical Aspects of Electron Ionization	293
5.1	Electron Ionization Ion Sources	294
5.1.1	Layout of an Electron Ionization Ion Source	294
5.1.2	Generation of Primary Electrons	296
5.1.3	Overall Efficiency and Sensitivity of an EI Ion Source	297
5.1.4	Optimization of Ion Beam Geometry	297
5.1.5	Mounting the Ion Source	299
5.2	Sample Introduction	300
5.2.1	Reservoir or Reference Inlet System	301
5.2.2	Direct Insertion Probe	302
5.2.3	Sample Vials for Use with Direct Insertion Probes	303
5.2.4	How to Run a Measurement with a Direct Insertion Probe	305
5.2.5	Automated Direct Insertion Probes	307

5.2.6	Fractionation When Using Direct Insertion Probes . . .	308
5.2.7	Direct Exposure Probe	310
5.3	Pyrolysis Mass Spectrometry	312
5.4	Gas Chromatograph	312
5.5	Liquid Chromatograph	313
5.6	Low-Energy Electron Ionization Mass Spectra	314
5.7	Analytes for EI	315
5.8	Mass Analyzers for EI	316
5.9	Mass Spectral Databases for EI	316
5.9.1	NIST/EPA/NIH Mass Spectral Database	317
5.9.2	Wiley Registry of Mass Spectral Data	318
5.9.3	Mass Spectral Databases: General Aspects	319
5.10	EI in a Nutshell	320
	References	321
6	Fragmentation of Organic Ions and Interpretation of EI Mass Spectra	325
6.1	Cleavage of a Sigma-Bond	326
6.1.1	Writing Conventions for Molecular Ions	326
6.1.2	σ -Bond Cleavage in Small Nonfunctionalized Molecules	328
6.1.3	Even-Electron Rule	329
6.1.4	σ -Bond Cleavage in Small Functionalized Molecules	331
6.2	Alpha-Cleavage	332
6.2.1	α -Cleavage of Acetone Molecular Ion	332
6.2.2	Stevenson's Rule	333
6.2.3	α -Cleavage of Nonsymmetrical Aliphatic Ketones	336
6.2.4	Acylium Ions and Carbenium Ions	338
6.2.5	α -Cleavage When Heteroatoms Belong to the Aliphatic Chain	339
6.2.6	α -Cleavage of Aliphatic Amines	340
6.2.7	Nitrogen Rule	342
6.2.8	α -Cleavage of Aliphatic Ethers and Alcohols	344
6.2.9	Charge Retention at the Heteroatom	345
6.2.10	α -Cleavage of Thioethers	346
6.2.11	α -Cleavage of Halogenated Hydrocarbons	347
6.2.12	Double α -Cleavage	349
6.2.13	Double α -Cleavage for the Identification of Regioisomers	350
6.3	Distonic Ions	351
6.3.1	Definition of Distonic Ions	351
6.3.2	Formation and Properties of Distonic Ions	352
6.3.3	Distonic Ions as Intermediates	353
6.4	Benzylic Bond Cleavage	354
6.4.1	Cleavage of the Benzylic Bond in Phenylalkanes	354

6.4.2	The Further Fate of $[C_6H_5]^+$ and $[C_7H_7]^+$	355
6.4.3	Isomerization of $[C_7H_8]^{++}$ and $[C_8H_8]^{++}$ Ions	357
6.4.4	Rings Plus Double Bonds	359
6.5	Allylic Bond Cleavage	360
6.5.1	Cleavage of the Allylic Bond in Aliphatic Alkenes	360
6.5.2	Methods for the Localization of the Double Bond	362
6.6	Cleavage of Non-activated Bonds	363
6.6.1	Saturated Hydrocarbons	363
6.6.2	Carbenium Ions	365
6.6.3	Very Large Hydrocarbons	367
6.7	Recognition of the Molecular Ion Peak	368
6.7.1	Rules for Identifying the Molecular Ion Peak	368
6.7.2	Common Neutral Losses	369
6.8	McLafferty Rearrangement	370
6.8.1	McL of Aldehydes and Ketones	371
6.8.2	Fragmentation of Carboxylic Acids and Their Derivatives	373
6.8.3	McL of Phenylalkanes	376
6.8.4	McL with Double Hydrogen Transfer	379
6.8.5	Benzyl Versus Benzoyl	380
6.8.6	Ubiquitous Plasticizers	381
6.9	Retro-Diels-Alder Reaction	381
6.9.1	Mechanism of the Retro-Diels-Alder Reaction	381
6.9.2	Widespread Occurrence of the RDA Reaction	383
6.9.3	RDA Reaction in Natural Products	384
6.10	Elimination of Carbon Monoxide	386
6.10.1	CO Loss from Phenols	386
6.10.2	CO and C_2H_2 Loss from Quinones	388
6.10.3	Fragmentation of Arylalkylethers	390
6.10.4	CO Loss from Transition Metal Carbonyl Complexes	393
6.10.5	CO Loss from Carbonyl Compounds	393
6.10.6	Differentiation Between Loss of CO, N_2 , and C_2H_4	394
6.11	Thermal Degradation Versus Ion Fragmentation	394
6.11.1	Decarbonylation and Decarboxylation	395
6.11.2	Retro-Diels-Alder Reaction	395
6.11.3	Loss of H_2O from Alkanols	395
6.11.4	EI Mass Spectra of Organic Salts	397
6.12	Alkene Loss from Onium Ions	398
6.12.1	McL of Onium Ions	399
6.12.2	Onium Reaction	403
6.13	Ion-Neutral Complexes	405
6.13.1	Evidence for the Existence of Ion-Neutral Complexes	406
6.13.2	Attractive Forces in Ion-Neutral Complexes	406

6.13.3	Criteria for Ion–Neutral Complexes	408
6.13.4	Ion–Neutral Complexes of Radical Ions	408
6.14	<i>Ortho</i> Elimination (<i>Ortho</i> Effect)	410
6.14.1	<i>Ortho</i> Elimination from Molecular Ions	411
6.14.2	<i>Ortho</i> Elimination from Even-Electron Ions	413
6.14.3	<i>Ortho</i> Elimination the Fragmentation of Nitroarenes	415
6.15	Heterocyclic Compounds	416
6.15.1	Saturated Heterocyclic Compounds	416
6.15.2	Aromatic Heterocyclic Compounds	421
6.16	Guide to the Interpretation of Mass Spectra	425
6.16.1	Summary of Rules	425
6.16.2	Systematic Approach to Mass Spectra	426
	References	427
7	Chemical Ionization	439
7.1	Basics of Chemical Ionization	440
7.1.1	Formation of Ions in Positive-Ion Chemical Ionization	440
7.1.2	Chemical Ionization Ion Sources	441
7.1.3	Chemical Ionization Techniques and Terms	442
7.1.4	Sensitivity of Chemical Ionization	442
7.2	Protonation in Chemical Ionization	443
7.2.1	Source of Protons	443
7.2.2	Methane Reagent Gas Plasma	444
7.2.3	CH ₅ ⁺ and Related Ions	446
7.2.4	Energetics of Protonation	446
7.2.5	Impurities of Higher <i>PA</i> than the Reagent Gas	447
7.2.6	Methane Reagent Gas PICI Spectra	448
7.2.7	Other Reagent Gases in PICI	450
7.3	Proton Transfer Reaction-Mass Spectrometry	453
7.3.1	Reagent ion Formation in PTR-MS	453
7.3.2	Analyte Ion Formation in PTR-MS	453
7.4	Charge Transfer Chemical Ionization	455
7.4.1	Energetics of CT	456
7.4.2	Reagent Gases for CTCI	457
7.4.3	Compound Class-Selective CTCI	458
7.4.4	Regio- and Stereoselectivity in CTCI	459
7.5	Negative-Ion Chemical Ionization	461
7.6	Electron Capture Negative Ionization	462
7.6.1	Ion Formation by Electron Capture	463
7.6.2	Energetics of Electron Capture	463

7.6.3	Creating Thermal Electrons	465
7.6.4	Appearance of ECNI Spectra	466
7.6.5	Applications of ECNI	467
7.7	Desorption Chemical Ionization	468
7.8	Atmospheric Pressure Chemical Ionization	469
7.8.1	Atmospheric Pressure Ionization	470
7.8.2	Atmospheric Pressure Chemical Ionization	471
7.8.3	Positive Ion Formation in APCI	472
7.8.4	Negative-Ion Formation in APCI	475
7.8.5	APCI Spectra	476
7.9	Atmospheric Pressure Photoionization	479
7.9.1	Ion Formation in APPI	480
7.9.2	APPI Spectra	482
7.10	Overview of CI, APCI, and APPI	486
	References	488
8	Field Ionization and Field Desorption	497
8.1	Evolution of Field Ionization and Field Desorption	497
8.2	Field Ionization Process	498
8.3	FI and FD Ion Sources	499
8.4	Field Emitters	501
8.4.1	Blank Metal Wires as Emitters	501
8.4.2	Activated Emitters	502
8.4.3	Emitter Temperature	503
8.4.4	Handling of Activated Emitters	504
8.5	Field Ionization Mass Spectrometry	505
8.5.1	Origin of $[M+H]^+$ Ions in FI-MS	506
8.5.2	Multiply-Charged Ions in FI-MS	506
8.5.3	Field-Induced Dissociation	507
8.5.4	Accurate Mass FI Spectra	507
8.5.5	Coupling Gas Chromatography to FI-MS	508
8.6	FD Spectra	509
8.6.1	Ion Formation by Field Ionization in FD-MS	509
8.6.2	Desorption of Preformed Ions in FD-MS	511
8.6.3	Cluster Ion Formation in FD-MS	513
8.6.4	FD-MS of Ionic Analytes	515
8.6.5	Temporal Evolution of FD Spectral Acquisition	517
8.6.6	Best Anode Temperature and Thermal Decomposition	518
8.6.7	FD-MS of Polymers	519
8.6.8	Negative-Ion Field Desorption – An Exotic Exception	521
8.6.9	Types of Ions in FD-MS	521
8.7	Liquid Injection Field Desorption Ionization	522
8.7.1	Positioning of the Capillary	523
8.8	General Properties of FI-MS and FD-MS	526

8.8.1	Sensitivity of FI-MS and FD-MS	526
8.8.2	Analytes and Practical Considerations for FI, FD, and LIFDI	526
8.8.3	Mass Analyzers for FI and FD	528
8.9	FI, FD, and LIFDI at a Glance	528
	References	530
9	Tandem Mass Spectrometry	539
9.1	Concepts of Tandem Mass Spectrometry	539
9.1.1	Tandem-in-Space and Tandem-in-Time	540
9.1.2	Pictograms for Tandem MS	542
9.1.3	Terminology for Tandem Mass Spectrometry	544
9.2	Metastable Ion Dissociation	544
9.3	Collision-Induced Dissociation	545
9.3.1	Effecting Collisions in a Mass Spectrometer	545
9.3.2	Energy Transfer During Collisions	546
9.3.3	Single and Multiple Collisions in CID	549
9.3.4	Time Scale of Ion Activating Processes	550
9.4	Surface-Induced Dissociation	552
9.5	Tandem MS on TOF Instruments	554
9.5.1	Utilizing a ReTOF for Tandem MS	554
9.5.2	Curved-Field Reflectron	557
9.5.3	Tandem MS on True Tandem TOF Instruments	558
9.6	Tandem MS with Magnetic Sector Instruments	559
9.6.1	Dissociations in the FFR Preceding the Magnetic Sector	559
9.6.2	Mass-analyzed Ion Kinetic Energy Spectra	560
9.6.3	Determination of Kinetic Energy Release	561
9.6.4	$B/E = Const.$ Linked Scan	562
9.6.5	Additional Linked Scan Functions	563
9.6.6	Multi-sector Instruments	564
9.7	Tandem MS with Linear Quadrupole Analyzers	566
9.7.1	Triple Quadrupole Mass Spectrometers	566
9.7.2	Scan Modes for Tandem MS with Triple Quadrupole Instruments	567
9.7.3	Penta Quadrupole Instruments	568
9.8	Tandem MS with the Quadrupole Ion Trap	569
9.9	Tandem MS with Linear Quadrupole Ion Traps	572
9.9.1	Tandem MS on QqLIT Instruments	572
9.9.2	Tandem MS on LITs with Radial Ejection	573
9.10	Tandem MS with Orbitrap Instruments	575
9.10.1	Higher-Energy C-Trap Dissociation	575
9.10.2	Extended LIT-Orbitrap Hybrid Instruments	577
9.11	Tandem MS with FT-ICR Instruments – Part I	578
9.11.1	Sustained Off-Resonance Irradiation-CID in ICR Cells	579

9.12	Infrared Multiphoton Dissociation	581
9.12.1	IRMPD in QITs and LITs	582
9.13	Electron Capture Dissociation	583
9.13.1	Principles of Electron Capture Dissociation	583
9.13.2	Peptide Ion Cleavages Upon ECD	584
9.14	Tandem MS with FT-ICR Instruments – Part II	586
9.14.1	IRMPD in FT-ICR-MS	586
9.14.2	Infrared Photodissociation Spectroscopy	587
9.14.3	Blackbody Infrared Radiative Dissociation	588
9.14.4	ECD for Tandem FT-ICR-MS	589
9.15	Electron Transfer Dissociation	591
9.16	Electron Detachment Dissociation	592
9.17	Special Applications of Tandem MS	594
9.17.1	Ion–Molecule Reactions in Catalytic Studies	594
9.17.2	Gas Phase Hydrogen–Deuterium Exchange	595
9.17.3	Determination of Gas Phase Basicities and Proton Affinities	596
9.17.4	Neutralization-Reionization Mass Spectrometry	598
9.18	Tandem Mass Spectrometry Condensed	599
	References	601
10	Fast Atom Bombardment	613
10.1	Brief Historical Sketch	613
10.2	Molecular Beam Solid Analysis	615
10.3	Ion Sources for FAB and LSIMS	616
10.3.1	FAB Ion Sources	616
10.3.2	LSIMS Ion Sources	619
10.3.3	FAB Probes	620
10.3.4	Sample Preparation for FAB and LSIMS	620
10.4	Ion Formation in FAB and LSIMS	621
10.4.1	Ion Formation from Inorganic Samples	621
10.4.2	Ion Formation from Organic Samples	622
10.5	Liquid Matrices for FAB and LSIMS	624
10.5.1	The Role of the Liquid Matrix	624
10.5.2	FAB Matrix Spectra: General Characteristics	626
10.5.3	Unwanted Reactions in FAB-MS	627
10.6	Applications of FAB-MS	627
10.6.1	FAB-MS of Analytes of Low to Medium Polarity	627
10.6.2	FAB-MS of Ionic Analytes	629
10.6.3	High-Mass Analytes in FAB-MS	630
10.6.4	Accurate Mass Measurements in FAB Mode	631
10.6.5	Low-Temperature FAB	633
10.6.6	FAB-MS and Peptide Sequencing	634
10.7	FAB and LSIMS: General Characteristics	635
10.7.1	Sensitivity of FAB-MS	635

10.7.2	Types of Ions in FAB-MS	636
10.7.3	Analytes for FAB-MS	636
10.7.4	Mass Analyzers for FAB-MS	637
10.7.5	Future Perspective for FAB and LSIMS	637
10.8	Massive Cluster Impact	638
10.9	²⁵² Californium Plasma Desorption	638
10.10	Ionization by Particle Impact at a Glance	640
	References	641
11	Matrix-Assisted Laser Desorption/Ionization	651
11.1	Ion Sources for LDI and MALDI	652
11.2	Ion Formation	654
11.2.1	Ion Yield and Laser Fluence	654
11.2.2	Effect of Laser Irradiation on the Surface	655
11.2.3	Temporal Evolution of a Laser Desorption Plume	657
11.2.4	Processes of Ion Formation in MALDI	660
11.2.5	“Lucky Survivor” Model of Ion Formation	660
11.3	MALDI Matrices	663
11.3.1	Role of the Solid Matrix	663
11.3.2	Matrices in UV-MALDI	663
11.3.3	Characteristics of MALDI Matrix Spectra	666
11.4	Sample Preparation	667
11.4.1	MALDI Target	667
11.4.2	Standard Sample Preparation	669
11.4.3	Cationization	670
11.4.4	Cation Exchange and the Need for Cation Removal	671
11.4.5	Anion Adducts	673
11.4.6	Solvent-Free Sample Preparation	673
11.4.7	Additional Methods of Sample Supply	675
11.5	Applications of LDI	675
11.6	Applications of MALDI	677
11.6.1	General Protein Analysis by MALDI-MS	677
11.6.2	Protein Fingerprints and MALDI Biotyping	678
11.6.3	Peptide Sequencing and Proteomics	681
11.6.4	Carbohydrate Analysis by MALDI-MS	686
11.6.5	Oligonucleotide Analysis by MALDI-MS	689
11.6.6	MALDI-MS of Synthetic Polymers	690
11.7	Special Surfaces to Mimic the Matrix Effect	694
11.7.1	Desorption/Ionization on Silicon	694
11.7.2	Nano-assisted Laser Desorption/Ionization	695
11.7.3	Further Variations of the MALDI Theme	696
11.8	MALDI Mass Spectral Imaging	697
11.8.1	Methodology of MALDI Imaging	697
11.8.2	Instrumentation for MALDI-MSI	698

11.8.3	Applications of MALDI-MSI	700
11.9	Atmospheric Pressure MALDI	703
11.10	Essentials of MALDI	705
	References	707
12	Electrospray Ionization	721
12.1	Route Leading to Electrospray Ionization	723
12.1.1	Atmospheric Pressure Ionization and Related Methods	723
12.1.2	Therospray	723
12.1.3	Electrohydrodynamic Ionization	724
12.1.4	Electrospray Ionization	725
12.2	Interfaces for Electrospray Ionization	726
12.2.1	Basic Design Considerations	726
12.2.2	Adaptation of ESI to Different Flow	727
12.2.3	Improved Electrospray Configurations	729
12.2.4	Advanced Atmospheric Pressure Interface Designs	730
12.2.5	Nozzle-Skimmer Dissociation	733
12.3	Nanoelectrospray	737
12.3.1	Practical Considerations for NanoESI	737
12.3.2	Spray Modes of NanoESI	739
12.3.3	Nanoelectrospray from a Chip	740
12.4	Ion Formation in ESI	741
12.4.1	Formation of the Electrospray Plume	741
12.4.2	Disintegration of Charged Droplets	744
12.4.3	Formation of Gas-Phase Ions from Charged Droplets	745
12.5	Multiply Charged Ions and Charge Deconvolution	747
12.5.1	Dealing with Multiply Charged Ions	747
12.5.2	Mathematical Charge Deconvolution	749
12.5.3	Computerized Charge Deconvolution	752
12.5.4	Hardware Charge Deconvolution	754
12.5.5	Controlled Charge Reduction in ESI	756
12.6	Applications of ESI-MS	757
12.6.1	ESI-MS of Small Molecules	757
12.6.2	ESI of Metal Complexes	758
12.6.3	ESI of Surfactants	759
12.6.4	Oligonucleotides, DNA, and RNA	759
12.6.5	ESI-MS of Oligosaccharides	762
12.6.6	Observing Supramolecular Chemistry at Work	762
12.6.7	High-Mass Proteins and Protein Complexes	765
12.7	Electrospray Roundup	766
	References	769

13	Ambient Desorption/Ionization	779
13.1	Concept of Ambient Desorption/Ionization	779
13.2	Desorption Electrospray Ionization	782
13.2.1	Experimental Setup for DESI	782
13.2.2	Parameters for DESI Operation	783
13.2.3	Mechanisms of Ion Formation in DESI	785
13.2.4	Analytical Features of DESI	787
13.3	Desorption Atmospheric Pressure Chemical Ionization	791
13.4	Desorption Atmospheric Pressure Photoionization	792
13.5	Other Methods Related to DESI	794
13.5.1	Desorption Sonic Spray Ionization	795
13.5.2	Extractive Electrospray Ionization	796
13.5.3	Electrospray-Assisted Laser Desorption/Ionization	797
13.5.4	Laser Ablation Electrospray Ionization	799
13.6	Rapid Evaporative Ionization Mass Spectrometry	800
13.6.1	Setup of Rapid Evaporative Ionization Mass Spectrometry	801
13.6.2	REIMS Spectra	801
13.6.3	REIMS in the Operating Room	801
13.7	Atmospheric Pressure Solids Analysis Probe	806
13.7.1	Setup of the Atmospheric Pressure Solids Analysis Probe	806
13.7.2	Atmospheric Pressure Solids Analysis Probe in Practice	806
13.8	Direct Analysis in Real Time	808
13.8.1	DART Ion Source	808
13.8.2	Positive Ion Formation in DART	810
13.8.3	Negative Ion Formation in DART	812
13.8.4	ADI Methods Related to DART	812
13.8.5	DART Configurations	813
13.8.6	Analytical Applications of DART	815
13.9	The World of Ambient Mass Spectrometry	820
	References	821
14	Hyphenated Methods	831
14.1	Chromatography	832
14.1.1	Chromatographic Column	832
14.1.2	Equilibrium of Adsorption and Desorption	833
14.1.3	Dead Time and Dead Volume	833
14.1.4	Retention Time	834
14.1.5	Elution and Eluate	834
14.1.6	Separation and Chromatographic Resolution	834
14.1.7	Detectors	836
14.1.8	Chromatograms	836
14.1.9	Gas Chromatography: Practical Considerations	837
14.1.10	Comprehensive Gas Chromatography	838

14.1.11	High-Performance Liquid Chromatography	840
14.2	Concept of Chromatography-Mass Spectrometry	844
14.2.1	Ion Chromatograms	845
14.2.2	Repetitive Acquisition of Mass Spectra During Elution	847
14.2.3	Selected Ion Monitoring and Targeted Analysis	849
14.2.4	Retrospective and Non-targeted Analysis	851
14.2.5	Selected Reaction Monitoring	852
14.3	Quantitation	854
14.3.1	Quantitation by External Standardization	856
14.3.2	Quantitation by Internal Standardization	857
14.3.3	Quantitation by Isotope Dilution	857
14.3.4	Retention Times of Isotopologs	858
14.4	Gas Chromatography-Mass Spectrometry	859
14.4.1	GC-MS Interfaces	859
14.4.2	Volatility and Derivatization	861
14.4.3	Column Bleed	862
14.4.4	Fast GC-MS	863
14.4.5	Multiplexing for Increased Throughput	864
14.4.6	Comprehensive Gas Chromatography-Mass Spectrometry	865
14.5	Liquid Chromatography-Mass Spectrometry	867
14.6	Ion Mobility Spectrometry-Mass Spectrometry	869
14.7	Tandem MS as a Complement to LC-MS	873
14.8	Ultrahigh-Resolution Mass Spectrometry	877
14.9	Summary of Hyphenated Techniques	878
	References	880
15	Inorganic Mass Spectrometry	889
15.1	Concept and Techniques of Inorganic MS	890
15.2	Thermal Ionization Mass Spectrometry	894
15.3	Spark Source Mass Spectrometry	896
15.4	Glow Discharge Mass Spectrometry	899
15.5	Inductively Coupled Plasma Mass Spectrometry	902
15.5.1	Laser Ablation ICP-MS	906
15.6	Secondary Ion Mass Spectrometry	907
15.6.1	Atomic SIMS	907
15.6.2	Instrumentation for Atomic SIMS	908
15.6.3	Molecular SIMS	910
15.6.4	Polyatomic Primary Ion Beams	911
15.7	Accelerator Mass Spectrometry	914
15.7.1	AMS Experimental Setup	914
15.7.2	AMS Facilities	915
15.7.3	Applications of AMS	916

15.8	Summary	917
	References	918
Appendix	927
A.1	Units, Physical Quantities, and Physical Constants	927
A.2	Isotopic Composition of the Elements	928
A.3	Carbon Isotopic Patterns	936
A.4	Chlorine and Bromine Isotopic Patterns	937
A.5	Silicon and Sulfur Isotopic Patterns	938
A.6	Reading Isotopic Patterns	939
A.7	Isotopologs and Accurate Mass	940
A.8	Characteristic Ions and Losses	941
A.9	Common Impurities	943
A.10	Identification of the Molecular Ion Peak	943
A.11	Rules for the Interpretation of Mass Spectra	944
A.12	Systematic Approach to Mass Spectra	945
A.13	Method Selection Guide	946
A.14	How to Recognize Cationization	948
A.15	Amino Acids	950
A.16	Nobel Prizes for Mass Spectrometry	951
A.17	One Hundred Common Acronyms	951
Index	955