

Contents

1 Introduction	1
1.1 What is mass spectrometry?	1
1.2 Atomic and molecular mass	2
1.3 What can mass spectrometry do?	3
1.4 The mass spectrometer	4
1.5 The mass spectrum	7
1.6 A brief history of mass spectrometry	10
1.7 Summary	12
1.8 Further reading	12
2 Methods of ionization	13
2.1 Introduction	13
2.2 Mechanisms of ion formation	14
2.3 Techniques for the ionization of vaporized samples	15
2.4 Desorption ionization techniques	24
2.5 Atmospheric pressure ionization techniques	30
2.6 Ambient ionization techniques	37
2.7 Summary	42
2.8 Exercises	42
2.9 Further reading	43
3 Methods of mass analysis	44
3.1 Introduction	44
3.2 Magnetic sector analysers	44
3.3 Quadrupole analysers	46
3.4 Time-of-flight analysers	48
3.5 Ion-trap analysers	50
3.6 Fourier transform ion cyclotron resonance analysers	51
3.7 Orbitrap analysers	53
3.8 Summary	55
3.9 Exercises	56
3.10 Further reading	56

4 Resolution, accurate mass, and sensitivity	57
4.1 Introduction	57
4.2 Resolving power and resolution	57
4.3 Accurate mass measurement	60
4.4 Sensitivity	66
4.5 Summary	70
4.6 Exercises	70
4.7 Further reading	72
5 Tandem mass spectrometry	73
5.1 Introduction	73
5.2 Ion dissociation	73
5.3 Methods of ion activation and dissociation for MS/MS	75
5.4 MS/MS instruments	80
5.5 MS/MS experiments	85
5.6 Summary	90
5.7 Exercises	90
5.8 Further reading	91
6 Interpretation of mass spectra	92
6.1 Introduction	92
6.2 Interpretation of EI mass spectra	92
6.3 Interpretation of mass spectra derived from protonation or deprotonation of the sample molecule	103
6.4 Summary	113
6.5 Exercises	113
6.6 Further reading	116
7 Separation techniques and quantification	117
7.1 Introduction	117
7.2 Why couple separation techniques to mass spectrometry?	117
7.3 Chromatography coupled to mass spectrometry	119
7.4 Liquid chromatography mass spectrometry (LC-MS)	124
7.5 Gas chromatography mass spectrometry (GC-MS)	129
7.6 Ion mobility separations and mass spectrometry	132
7.7 Quantitation by mass spectrometry	134
7.8 Summary	139

7.9 Exercises	140
7.10 Further reading	140

8 Mass spectrometry applications 141

8.1 Introduction	141
8.2 Mass spectrometry applications in the environment and sport	141
8.3 Small-molecule mass spectrometry in biology and medicine	148
8.4 Analysis of proteins	158
8.5 Mass spectrometry imaging	168
8.6 Summary	171
8.7 Exercises	171
8.8 Further reading	172

Glossary 173

Index 177