TABLE OF CONTENTS

Preface xvii

Chapter 0: Some Philosophical Discourse on the Use of Computers in Chemistry 1

0.1 Initial Considerations 1
0.2 Opinions of computing environments 3
0.3 How topics will be presented in this book 4
0.4 Type of calculations to be stressed 4
0.5 A chemically-oriented view of computers and computation 5
0.6 A strictly computer-oriented problem 5
0.7 Some other thoughts 6
0.8 A comment on notation 7

PART I: A general look at how computers can be used in scientific applications

Chapter 1: A General Presentation of Various Mathematical Approaches 11

1.1 Analytical approaches to mathematical problems 11
1.1.1 Why an analytical method is usually the best way to proceed 11
1.1.2 One major exception to the above rules 12
1.2 The writing of mathematical expressions 12
1.2.1 Some very basic rules 12
1.2.2 Stating the "rules" another way 14
1.3 Ways to write equations 16
1.3.1 The grammar and syntax of mathematical expressions 17
1.3.2 Efficiency of evaluation vs. ease of understanding 18
1.3.3 A note on problems and exercises 19
1.4 Developing analytical methods 22
1.4.1 Reference works you can consult for sources of equations (and other reference works specifically useful for computational purposes) 22
1.4.1.1 "Mathematical formularies" 23

1.4.1.2 Integral and derivative tables 23
1.4.1.3 Textbooks 24
1.4.1.4 Computer manuals 24
1.4.1.5 Computer language manuals 25
1.4.1.6 Manuals for specific programs 27
1.4.2 Acquiring an algebraic "bag of tricks" 28
1.4.2.1 The method of partial fractions 29
1.4.2.2 Some hints about trigonometric functions 35
1.4.3 Derivatives, differentials, and integrals 42
1.4.3.1 Derivatives and differentials 43
1.4.3.2 One important application of derivatives (and a word of warning) 51
1.4.3.3 A very short review of the integral calculus 55
1.4.4 A review of complex numbers 59
1.5 Summary 65

Chapter 2: A Look at the Numerical (or Computational) Approach 67

2.1 Algorithms 67
2.1.1 Some points concerning algorithmic efficiency 68
2.2 Computer programming: The art of using algorithms 71
2.3 Some rules for good computer programming 73
2.3.1 Stating algorithms in a form best suited to programming 73
2.3.2 Structured programming 75
2.3.3 Size vs. speed in programming 78
2.3.4 User-friendliness 78
2.3.4.1 The computer languages to be used in this book 82
2.3.4.2 A further word about user friendliness in the context of structured programming 94
2.3.5 The use of remarks (comments) in programming 98
2.3.6 Summary 99
2.4 An overview of computer applications 100
2.4.1 A main application: Calculation 100
2.4.2 Data handling and manipulation 101
2.4.2.1 Sorting 101

2.4.2.2 A small complication to sorting: Companion arrays 112
2.4.2.3 Searching 113
2.5 Some application programs 115
2.5.1 The most important application program: DOS 116
2.5.2 Word processors 117
2.5.2.1 Word processors and program writing 123
2.5.3 Database programs 123
2.5.4 Spreadsheets 125
2.5.5 Some final thoughts concerning specific applications of computers 126
2.6 Computers--Types and uses 127
2.6.1 Microcomputers 130
2.6.2 Minicomputers 131
2.6.3 Main frame computers 132
2.6.4 Using computers together: Networking 133
2.6.5 Some types of useful hardware used with computers 134
2.6.5.1 Keyboards and monitors 134
2.6.5.2 Printers 136
2.6.5.3 Disk drives and casette tape drives 137
2.6.5.4 Some other devices 139
2.6.5.5 System configurations: What do you need? 143
2.6.6 Programming languages: How we "talk" to computers 144
2.6.6.1 Machine language 144
2.6.6.2 Assembly language 144
2.6.6.3 High level languages not used in this book 147
2.6.6.4 The BASIC programming language 150
2.7 Some problems encountered when using computers 151
2.8 Summary 153

Chapter 3: Geometrical Approaches to Problem Solving and an Introduction to Computer Graphics 157

3.1 Some initial considerations 157
3.2 How to draw a graph 158
3.3 An aside on coordinates used in computer plotting 194
3.4 Plotting in three dimensions 199

3.5 Contour plotting 220
3.6 Summary 231

Chapter 4: [An Example of] A Complete Program Package for People who Prefer to Use an Interpreter 233

PART II: A detailed look at some mathematical and numerical approaches

Chapter 5: Analytical and Numerical Methods for the Solution of Algebraic Equations 257

5.1 Initial considerations 257
5.2 Some elementary analytical methods 258
5.2.1 Some basics concerning roots of polynomials 258
5.2.2 Quadratic equations 260
5.2.3 Cubic equations 266
5.2.4 Quartic equations 272

Chapter 6: A More Complete Introduction to Numerical Methods for Solving Algebraic Equations 275

6.1 Initial considerations 275
6.2 The iterative (or simple iterative) method 276
6.3 F(x) = 0 methods without derivatives 284
6.3.1 The bisection method 292
6.3.2 The method of false position 297
6.3.3 The secant method 300
6.4 The Newton-Raphson method (or how to use derivatives) 303
6.5 A reminder of some programming practices 308
6.6 Some comments regarding roots of polynomials 308

Chapter 7: An Extensive Example of the Use of Numerical Root-Seeking Methods: The Calculation of pH in General Acid-Base Equilibria 315

7.1 Initial considerations 315
7.2 The calculation of pH for weak acids titrated by strong bases 315
7.2.1 A basic definition of the problem 315
7.2.1.1 The monoprotic acid case--setting up the equations to be solved 317
7.2.1.2 The case of diprotic acids titrated by a strong base 319
7.2.1.3 The general case of an n-protic acid titrated by a strong base 320
7.3 Writing a program to calculate the hydrogen ion concentration for a mixture of weak acid and strong base 321
7.4 The requirements of a calling routine for the subroutines of section 7.3 328

Chapter 8: Numerical Methods for Getting Derivatives and Integrals of Mathematical Functions 345

8.1 Some introductory remarks 345
8.2 Numerical differentiation 346
8.3 Numerical integration 349
8.3.1 Trapezoidal and Simpson quadrature 350
8.3.2 Gaussian quadrature and some other advanced methods of integration 356
8.3.3 Some applications of numerical integration 366

Chapter 9: Some Special Functions and How to Evaluate Them 371

9.1 Some introductory remarks with regard to special functions 371
9.2 The gamma function 371
9.3 Legendre and Laguerre polynomials 374

Chapter 10: Determinants and Matrices 383

10.1 Some introductory remarks 383
10.2 Determinants 383

10.3 Determinants and simultaneous equations: Cramer's rule 393
10.4 Matrices 395
10.5 Matrix inversion 415
10.6 Orthogonal matrices 425
10.7 Matrix diagonalization 427
10.7.1 The Jacobi method of matrix diagonalization 429
10.7.2 The Givens-Householder method 433
10.8 Some useful tricks applying matrix diagonalization 443

Chapter 11: Differential Equations 447

11.1 Some initial considerations 447
11.2 Numerical solution of differential equations 450

Chapter 12: Model Fitting and Data Analysis 461

12.1 Some initial considerations 461
12.2 Model fitting 461
12.3 Regression analysis 463
12.4 Linear regression 465
12.4.1 Linear regression with a single parameter 465
12.4.2 The two-parameter case: Best fit to a straight line 468
12.4.3 General linear regression 474
12.5 The artificial generation of test data sets 477
12.6 Direct search methods 482
12.7 Linearization 493
12.8 Gradient search methods 494

Chapter 13: Monte Carlo Methods 509

13.1 Some introductory comments 509
13.2 Definite integrals and Monte Carlo methods 510
13.2.1 Probability distributions 510
13.2.2 The evaluation of definite integrals by Monte Carlo methods 512
13.3 An aside on the quality of random distributions 518

PART III: Some computer applications and long program listings

Chapter 14: Molecular Graphics 523

Chapter 15: The Generation and Plotting of Molecular Spectra. NMR Spectra Presented as an Example 575

Chapter 16: Fourier Transforms 613

APPENDICES

Appendix A: A Short Glossary of Mathematical and Computing Terms 649

Appendix B: A Short Discussion of QB87 (Microsoft QuickBASIC) 655

Appendix C: Some Useful Differentials 667

BIBLIOGRAPHY AND INDEX

Bibliography 669

Index 675