Table of Contents

1 The Basics: Mathematical Functions, Rearranging Equations and Handling Units 3

- 1.1: Reversible Reactions, Reversible Mathematics 03
- 1.2: An Introduction to Mathematical Operations 05
- 1.3: Treating Both Sides Fairly: The Nature of Equality 15
- 1.4: Dimensional Analysis 19
- 1.5: Interconverting Units 25
- 1.6 Summary 27

2 Probability and Statistics in Chemistry 35

- 2.1: Probability in Chemical Kinetics 36
- 2.2: Flipping Coins, Filling Reactions 37
- 2.3: Standard Distributions and Standard Deviations 49
- 2.4: Summary 58

3 Experimental Uncertainty and Significant Figures: What Are the Bounds of Experimental Error? 63

- 3.1: Accuracy and Precision 63
- 3.2: Managing Significant Figures 66
- 3.3: The Standard Error 74
- 3.4: Combining Uncertainties 77
- 3.5: Identifying Outliers in a Single Data Series 85
- 3.6: Comparing Data Series—Student's *t* Test 89
- 3.7: Summary 94

4 Tables and Graphs – Presenting and Analysing Experimental Data 103

- 4.1: Recording Data 103
- 4.2: Straight-line Graphs: '$y = mx + c$' 106
- 4.3: Determining Gradients and Intercepts 112
- 4.4: Uncertainties in Straight-line Graphs 115
- 4.5: Plotting Experimental Data 118
- 4.6: Summary 121

5 Trigonometry and Coordinate Systems: Describing Molecular Positions 131

- 5.1: Determination of Molecular Distances 131
- 5.2: Molecular Geometry: Molecular Spectroscopy 142
- 5.3: Coordinate Systems 146
- 5.4: Summary 154

6 Vectors, Directions and Crystal Structures 161

- 6.1: A Brief Introduction to the Vector 161
- 6.2: Two (and Higher) Dimensional Vectors 163
- 6.3: Vector Addition, Subtraction and Scaling 165
- 6.4: Vector Multiplication: Work Done and Torque 169
- 6.5: Vectors in Crystallography 179
- 6.6: Summary 181

7 Calculus 1, Differentiation: Mean Speeds and Equilibrium Separations 185

7.1: Rates of Change 185
7.2: Differentiating Special Functions 195
7.3: Finding the Maximum and the Minimum 198
7.4: More Advanced Differentiation 203
7.5: Partial Differentiation of Multiple Variables 210
7.6: Summary 213

8 Calculus 2, Integration: Reaction Kinetics and Rate Laws 223

8.1: The Need for an Inverse Function 223
8.2: Integration—Exploring the Harmonic Oscillator 224
8.3: Chemical Kinetics—Determining the Rate Law 230
8.4: Calculating Thermodynamic Work 235
8.5: Integration in Context 245
8.6: Summary 254

9 Complex Numbers: Quantum Mechanics and Solving the Schrödinger Equation 261

9.1: Complex Numbers in Chemistry 261
9.2: Introduction to Complex Numbers 263
9.3: Arithmetic With Complex Numbers 266
9.4: Alternative Representations of Complex Numbers 269
9.5: Complex Numbers and Wave Functions 274
9.6: Summary 277

Appendix: The Mathematical Toolkit 288

Reading List 301

Index 302