

Chemical Calculations

Mathematics for Chemistry

Third Edition

Paul C. Yates

Deputy Director of Learning, Teaching and Scholarship



CRC Press

Taylor & Francis Group

Boca Raton London New York

CRC Press is an imprint of the
Taylor & Francis Group, an Informa business

KATALOG

Contents

Preface.....	xiii
Acknowledgement.....	xv
Author.....	xvii

Chapter 1	Fundamentals.....	1
1.1	Introduction	1
1.2	Positive and Negative Numbers.....	1
1.2.1	Addition	1
1.2.2	Subtraction	2
1.2.3	Multiplication.....	3
1.2.4	Division.....	5
1.3	Precedence in Equations.....	6
1.4	Rearranging Equations.....	9
1.5	Fractions.....	11
1.5.1	Identical Fractions.....	11
1.5.2	Addition and Subtraction	13
1.5.3	Multiplication.....	14
1.5.4	Division.....	15
1.6	Indices.....	16
1.6.1	Multiplication.....	17
1.6.2	Division.....	17
1.6.3	Raising to a Power.....	18
1.6.4	Roots.....	19
1.6.5	Negative Powers.....	19
1.7	Standard Form	20
	Exercises.....	21
	Problems.....	23

Chapter 2	Experimental Techniques.....	27
2.1	Introduction	27
2.2	Measurement in Chemistry.....	28
2.2.1	Decimal Places.....	28
2.2.2	Significant Figures.....	29
2.2.3	Combining Quantities.....	31
2.3	Stoichiometric Calculations	33
2.3.1	Multiplication and Division by an Integer.....	33
2.4	Uncertainty in Measurement	36
2.4.1	Types of Uncertainty	37
2.4.2	Combining Uncertainties.....	38
2.4.2.1	Determining the Maximum Possible Uncertainty.....	38
2.4.2.2	Determining the Maximum Probable Uncertainty.....	39

2.4.3	Statistical Treatment of Uncertainties	44
2.4.3.1	Statistics Using a Calculator	48
2.4.3.2	Statistics Using a Spreadsheet	51
	Exercises	52
	Problems	55
Chapter 3	Thermodynamics	57
3.1	Fractions and Indices in the Equilibrium Constant	57
3.2	Bond Enthalpies	58
3.2.1	Rearranging Equations	59
3.3	The Born-Haber Cycle	60
3.3.1	Combining Uncertainties	60
3.4	Heat Capacity	63
3.4.1	Expansion of Brackets	64
3.4.2	Polynomial Expressions	65
3.4.3	Functions	69
3.5	Clapeyron Equation	70
3.5.1	Differentiation	71
3.6	Clausius-Clapeyron Equation	79
3.6.1	Logarithms	80
3.6.2	The Equation of a Straight Line	83
3.6.3	Plotting Graphs	85
3.6.4	Plotting Graphs Using a Spreadsheet	89
3.7	The Ideal Gas Equation	90
3.7.1	Dimensional Analysis	90
3.7.2	Interconversion of Units	91
3.7.3	Constants and Variables	93
3.7.4	Proportion	95
3.7.5	Functions of Two Variables	97
3.7.6	Partial Differentiation	99
3.7.7	The Differential	103
3.8	The van der Waals Equation	105
3.8.1	Expansion of Brackets	106
3.8.2	Combining Limits	107
3.9	Equilibrium Constants	109
3.9.1	Solving Quadratic Equations Using a Formula	112
3.9.2	Solving Quadratic Equations Iteratively	114
	Exercises	115
	Problems	118
Chapter 4	Solution Chemistry	123
4.1	Introduction	123
4.2	Concentration of Solutions	123
4.2.1	Concentration of a Solution	123
4.2.2	Dilution of a Solution	125
4.3	Activity	126
4.4	Molality	127
4.4.1	Proportion	127

4.5	Raoult's Law.....	128
4.5.1	Straight Line Graphs.....	128
4.5.2	Proportion.....	130
4.6	The Debye-Hückel Equation.....	131
4.6.1	Logarithms.....	132
4.7	Ostwald's Dilution Law.....	134
4.7.1	Discontinuities.....	135
4.8	Partial Molar Volumes.....	137
4.8.1	Functions.....	137
4.8.2	Stationary Points.....	139
	Exercises.....	142
	Problems.....	145

Chapter 5	Kinetics.....	149
5.1	Introduction.....	149
5.2	Using a Rate Equation.....	149
5.3	Rates of Change.....	150
5.4	Zero-Order Reactions.....	153
5.4.1	Integration.....	154
5.5	First-Order Reactions.....	161
5.5.1	Integration of $\frac{1}{x}$	161
5.5.2	Rules of Combining Logarithms.....	161
5.6	Second-Order Reactions.....	169
5.6.1	Partial Fractions.....	176
5.6.2	Differentiation of Logarithmic Functions and Integration of Fractions.....	178
5.7	The Arrhenius Equation.....	185
5.7.1	The Exponential Function.....	185
5.7.2	Inverse Functions.....	185
5.8	The Steady State Approximation.....	192
5.8.1	Simultaneous Equations.....	192
	Exercises.....	196
	Problems.....	199

Chapter 6	Structural Chemistry.....	201
6.1	Introduction.....	201
6.2	Packing Fractions of Atoms in Metals.....	201
6.3	Arrangement of Atoms in Crystals.....	204
6.3.1	Pythagoras' Theorem.....	204
6.3.2	Pythagoras' Theorem in Three Dimensions.....	206
6.4	Bragg's Law.....	207
6.4.1	Trigonometry.....	208
6.4.2	Inverses of Trigonometric Functions.....	211
6.5	The Unit Cell.....	213
6.5.1	Unit Vectors.....	213
6.5.2	Addition and Subtraction of Vectors.....	213
6.5.3	Multiplication of Vectors.....	215
6.6	X-Ray Diffraction.....	223

	6.6.1 Complex Numbers.....	224
6.7	Symmetry Operators.....	228
	6.7.1 Matrices.....	233
	Exercises.....	235
	Problems.....	
Chapter 7	Quantum Mechanics.....	239
	7.1 Introduction.....	239
	7.2 Energy Level Transitions and Appropriate Precision.....	240
	7.3 The Photon.....	241
	7.3.1 Mathematical Relationships.....	244
	7.4 Forces between Atoms.....	244
	7.4.1 Proportionality.....	246
	7.4.2 Stationary Points.....	250
	7.5 Particle in a Box.....	250
	7.5.1 Complex Numbers.....	252
	7.5.2 Sequences.....	253
	7.5.3 Inverse Functions.....	255
	7.5.4 Differentiation of Fractional Indices.....	257
	7.5.5 Use of Standard Integrals.....	260
	7.6 The Free Particle.....	260
	7.6.1 The Complex Conjugate.....	261
	7.6.2 The Modulus of a Complex Number.....	263
	7.7 The Hydrogen Atom Wavefunction.....	263
	7.7.1 Differentiation of a Product.....	265
	7.7.2 Integration by Parts.....	266
	7.7.3 Calculus of the Exponential Function.....	271
	7.7.4 Multiple Integration.....	273
	7.7.5 Calculus of the Trigonometric Functions.....	276
	7.8 The Helium Atom.....	276
	7.8.1 Stationary Points.....	278
	7.9 Hückel Theory.....	278
	7.9.1 Determinants.....	281
	Exercises.....	284
	Problems.....	
Chapter 8	Spectroscopy.....	289
	8.1 Introduction.....	289
	8.2 Calculation of Dipole Moments.....	290
	8.3 Dipole and Quadrupole Moments.....	293
	8.4 Electromagnetic Radiation.....	293
	8.4.1 Direct and Inverse Proportion.....	296
	8.5 The Beer-Lambert Law.....	297
	8.5.1 Rules of Logarithms.....	298
	8.6 Rotational Spectroscopy.....	298
	8.6.1 Sequences.....	301
	8.7 Vibrational Spectroscopy.....	305
	8.8 Rotation-Vibration Spectroscopy.....	307
	8.9 Nuclear Magnetic Resonance Spectroscopy.....	

8.9.1	Pascal's Triangle	307
8.10	Fourier Transform Spectroscopy	311
8.10.1	Introduction to Fourier Transforms	311
	Exercises	314
	Problems	318
Chapter 9	Statistical Mechanics	321
9.1	Introduction	321
9.2	Molecular Energy Distributions	321
9.3	Configurations	322
9.3.1	Factorials	322
9.4	The Boltzmann Equation	325
9.4.1	Differentiation of Logarithms	326
9.4.2	Differentiation of Products	326
9.5	The Partition Function	329
9.5.1	Integration by Substitution	329
9.5.2	Calculating a Series Using a Spreadsheet	334
	Exercises	336
	Problems	339
Appendix A: Units		343
Appendix B: Physical Constants		345
Answers to Exercises		347
Answers to Problems		355
Chemical Index		361
Mathematical Index		367