

Contents

Atkins + de Paula

9th Edition

Fundamentals

	1
F.1 Atoms	1
F.2 Molecules	2
F.3 Bulk matter	4
F.4 Energy	6
F.5 The relation between molecular and bulk properties	7
F.6 The electromagnetic field	9
F.7 Units	10
Exercises	13

PART 1 Equilibrium

1 The properties of gases

	19
The perfect gas	19
1.1 The states of gases	19
1.2 The gas laws	23
11.1 Impact on environmental science: The gas laws and the weather	28
Real gases	29
1.3 Molecular interactions	30
1.4 The van der Waals equation	33
Checklist of key equations	37
Discussion questions	38
Exercises	38
Problems	39
Mathematical background 1: Differentiation and integration	42

2 The First Law

	44
The basic concepts	44
2.1 Work, heat, and energy	45
2.2 The internal energy	47
2.3 Expansion work	49
2.4 Heat transactions	53
2.5 Enthalpy	56
12.1 Impact on biochemistry and materials science: Differential scanning calorimetry	62
2.6 Adiabatic changes	63

Thermochemistry

	65
2.7 Standard enthalpy changes	65
12.1 Impact on biology: Food and energy reserves	70
2.8 Standard enthalpies of formation	71
2.9 The temperature dependence of reaction enthalpies	73
State functions and exact differentials	74
2.10 Exact and inexact differentials	74
2.11 Changes in internal energy	75
2.12 The Joule-Thomson effect	79
Checklist of key equations	83
Further information 2.1: Adiabatic processes	84
Further information 2.2: The relation between heat capacities	84
Discussion questions	85
Exercises	85
Problems	88
Mathematical background 2: Multivariate calculus	91
MB2.1 Partial derivatives	91
MB2.2 Exact differentials	92

3 The Second Law

	94
The direction of spontaneous change	95
3.1 The dispersal of energy	95
3.2 Entropy	96
13.1 Impact on engineering: Refrigeration	103
3.3 Entropy changes accompanying specific processes	104
3.4 The Third Law of thermodynamics	109
13.2 Impact on materials chemistry: Crystal defects	112
Concentrating on the system	113
3.5 The Helmholtz and Gibbs energies	113
3.6 Standard molar Gibbs energies	118
Combining the First and Second Laws	121
3.7 The fundamental equation	121
3.8 Properties of the internal energy	121
3.9 Properties of the Gibbs energy	124
Checklist of key equations	128
Further information 3.1: The Born equation	128
Further information 3.2: The fugacity	129

Discussion questions	130	6 Chemical equilibrium	209
Exercises	131	Spontaneous chemical reactions	209
Problems	132	6.1 The Gibbs energy minimum	210
4 Physical transformations of pure substances	135	16.1 Impact on biochemistry: Energy conversion in biological cells	211
Phase diagrams	135	6.2 The description of equilibrium	213
4.1 The stabilities of phases	135	The response of equilibria to the conditions	221
4.2 Phase boundaries	137	6.3 How equilibria respond to changes of pressure	221
4.3 Three representative phase diagrams	140	6.4 The response of equilibria to changes of temperature	223
14.1 Impact on technology: Supercritical fluids	142	16.2 Impact on technology: Supramolecular chemistry	226
Thermodynamic aspects of phase transitions	143	Equilibrium electrochemistry	227
4.4 The dependence of stability on the conditions	143	6.5 Half-reactions and electrodes	228
4.5 The location of phase boundaries	146	6.6 Varieties of cells	229
4.6 The Ehrenfest classification of phase transitions	149	6.7 The cell potential	230
Checklist of key equations	152	6.8 Standard electrode potentials	23
Discussion questions	152	6.9 Applications of standard potentials	23
Exercises	153	16.3 Impact on technology: Species-selective electrodes	23
Problems	154	Checklist of key equations	24
5 Simple mixtures	156	Discussion questions	24
The thermodynamic description of mixtures	156	Exercises	2
5.1 Partial molar quantities	157	Problems	2
5.2 The thermodynamics of mixing	161	PART 2 Structure	2
5.3 The chemical potentials of liquids	164	7 Quantum theory: introduction and principles	
The properties of solutions	167	The origins of quantum mechanics	
5.4 Liquid mixtures	167	7.1 Energy quantization	
5.5 Colligative properties	169	7.2 Wave-particle duality	
15.1 Impact on biology: Osmosis in physiology and biochemistry	175	17.1 Impact on biology: Electron microscopy	
Phase diagrams of binary systems	176	The dynamics of microscopic systems	
5.6 Vapour pressure diagrams	176	7.3 The Schrödinger equation	
5.7 Temperature-composition diagrams	179	7.4 The Born interpretation of the wavefunction	
5.8 Liquid-liquid phase diagrams	181	Quantum mechanical principles	
5.9 Liquid-solid phase diagrams	185	7.5 The information in a wavefunction	
15.2 Impact on materials science: Liquid crystals	188	7.6 The uncertainty principle	
Activities	190	7.7 The postulates of quantum mechanics	
5.10 The solvent activity	190	Checklist of key equations	
5.11 The solute activity	191	Further information 7.1: Classical mechanics	
5.12 The activities of regular solutions	194	Discussion questions	
5.13 The activities of ions in solution	195	Exercises	
Checklist of key equations	198	Problems	
Further information 5.1: The Debye-Hückel theory of ionic solutions	199		
Discussion questions	200		
Exercises	201		
Problems	204		