

Revised Edition

ELEMENTARY ORGANIC SPECTROSCOPY

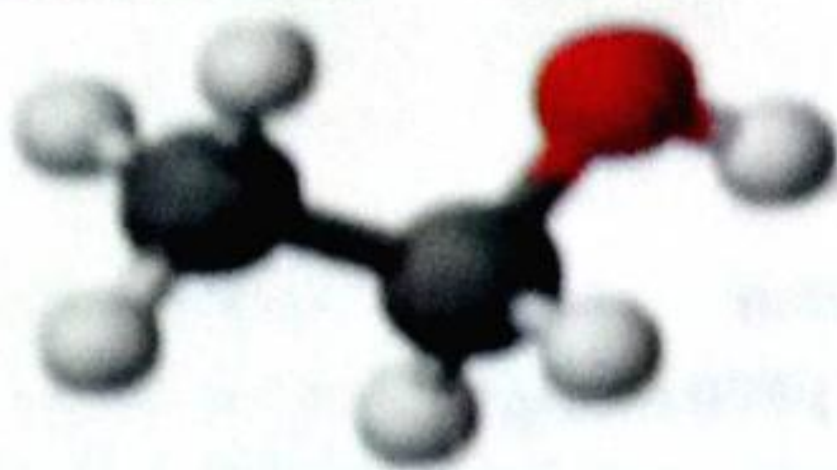
PRINCIPLES AND CHEMICAL APPLICATIONS

FOR B.Sc. (HONS.), POSTGRADUATE STUDENTS OF ALL
INDIAN UNIVERSITIES AND COMPETITIVE EXAMINATIONS

Y.R. SHARMA



S. CHAND

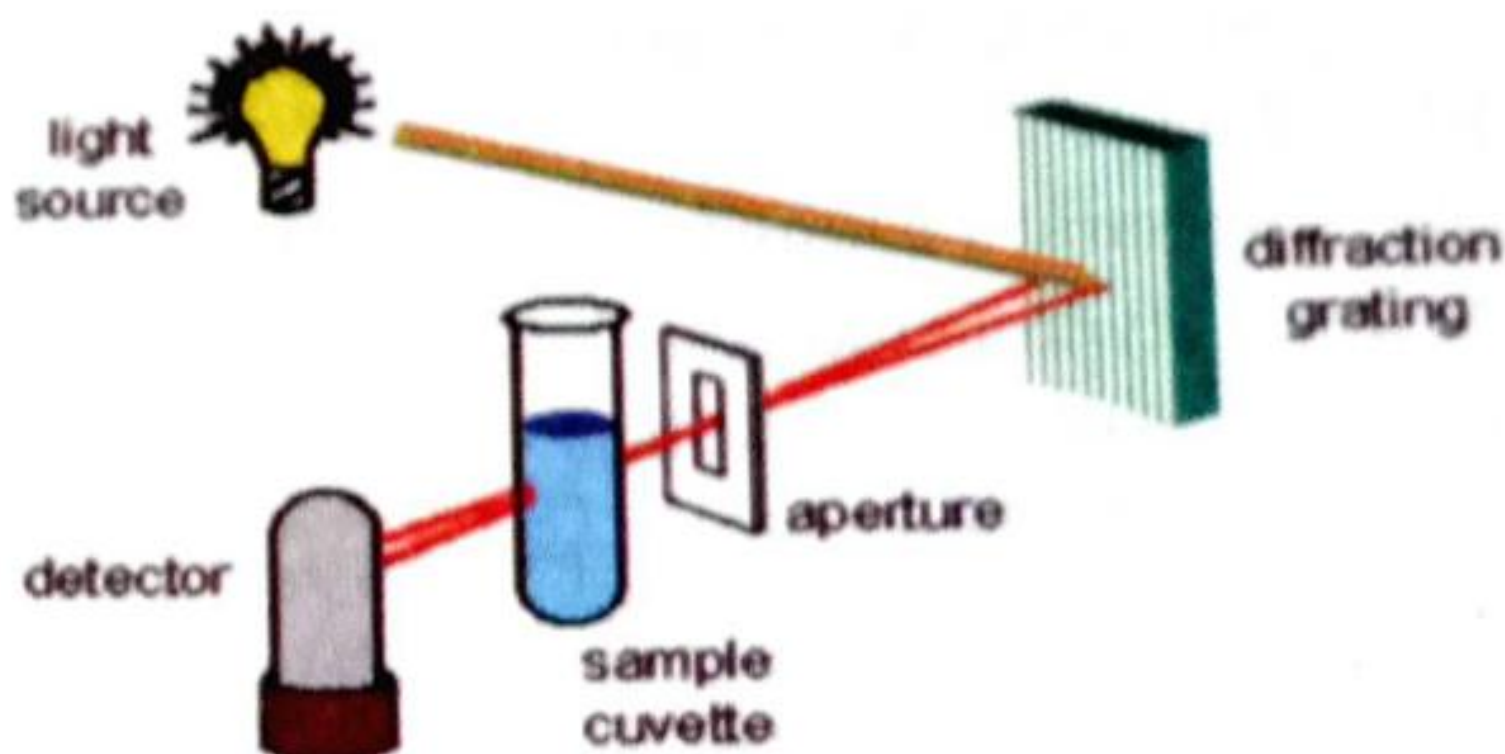


CHAPTER 1: INTRODUCTION

1.1	Electro-magnetic radiations	1
1.2	Units	3
1.3	Electromagnetic Spectrum and Absorption of Radiations	5
	Further Readings	8
	Review Questions	8
	Multiple Choice Questions	8

CHAPTER 2: ULTRA-VIOLET AND VISIBLE SPECTROSCOPY

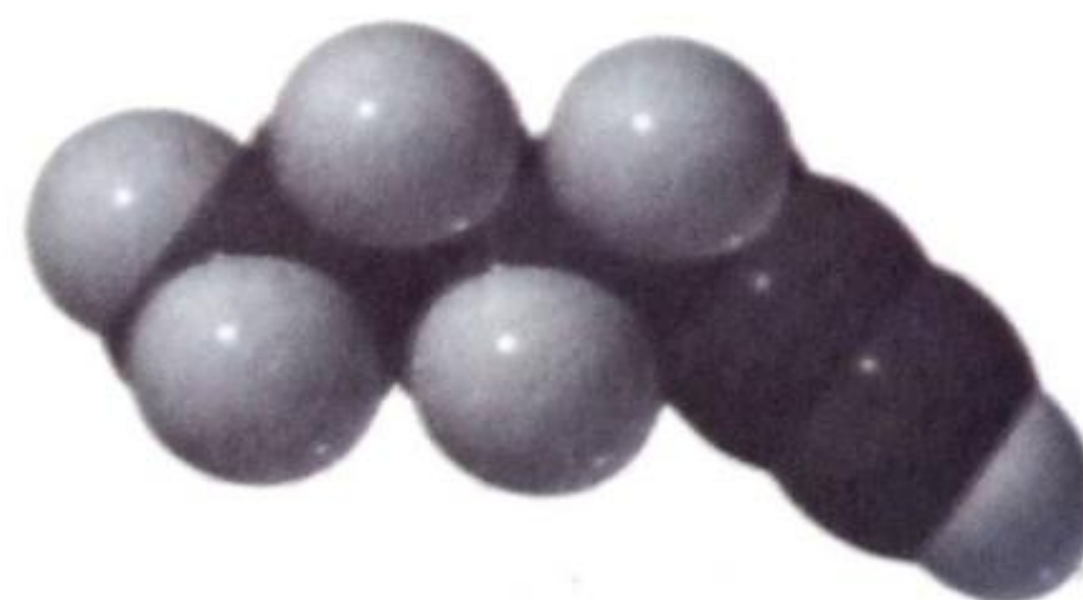
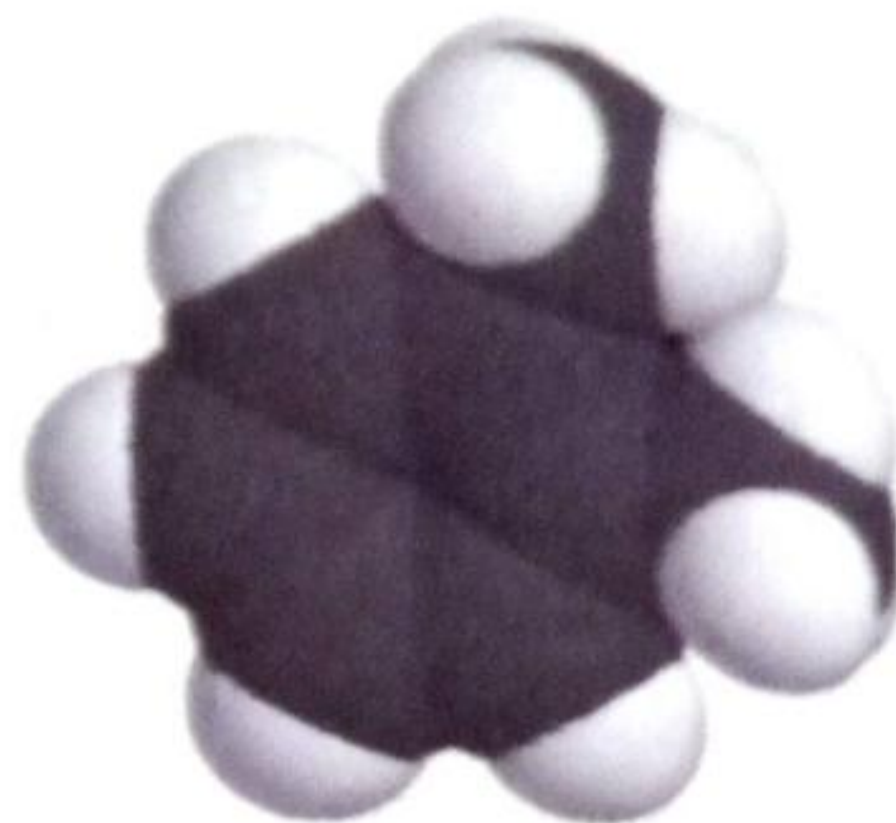
2.1	Introduction	11
2.2	The Absorption Laws	12
2.3	Measurement of Absorption Intensity	16
2.4	Instrumentation	16
2.5	Formation of Absorption Bands	18
2.6	Theory of Electronic Spectroscopy	19
2.7	Types of Electronic Transitions	19
2.8	Transition Probability	22
2.9	The Chromophore Concept	23
2.10	Auxochrome	24
2.11	Absorption and Intensity shifts	25
2.12	Types of Absorption bands	26
2.13	Solvent Effects	27
2.14	Effect of Temperature and Solvent on the Fineness of Absorption Band	29
2.15	Conjugated dienes	30
2.16	Woodward-fieser Rules for Calculating Absorption Maximum in Dienes	33
2.17	Distortion of the Chromophore	37
2.18	Poly-enes and Poly-yne	38
2.19	Ultra-violet Absorption in α , β -unsaturated Carbonyl Compounds	40
2.20	Woodward-fieser rules for Calculating Absorption Maximum in α , β -unsaturated carbonyl compounds	42
2.21	Compounds with N to O Bonds	47
2.22	Benzene and its Derivatives	47
2.23	Rules for Calculating Absorption Maximum for Derivatives of Acyl-benzenes	48
2.24	Absorption Spectra of Condensed Ring Systems	49
2.25	Heterocyclic Compounds	49
2.26	Steric Hindrance and Coplanarity	51
2.27	Fluorescence and Phosphorescence	52
2.28	Electronic Transitions for Charge Transfer Complexes	53



2.29	Study of Keto-enol Tautomerism	
2.30	Applications of ultra-violet Spectroscopy	
2.31	Important Features in Electronic Spectroscopy	
2.32	Important Terms and Definitions in Ultraviolet Spectroscopy	
2.33	Short Questions with Answers	
	Further Readings	
	Review Questions	
	Multiple Choice Question	

CHAPTER 3: INFRA-RED SPECTROSCOPY

3.1	Introduction	
3.2	Principle of Infra-red Spectroscopy	
3.3	Theory—Molecular vibrations	
3.4	Vibrational Frequency	
3.5	Number of fundamental vibrations	
3.6	Selection Rules	
3.7	Factors Influencing Vibrational Frequencies	
3.8	Scanning of infra-red Spectrum	
3.9	Sampling Techniques	
3.10	Finger Print Region	
3.11	Spectral Features of Some Classes of Organic Compounds	
3.11	A Hydrocarbons	
3.11	A ₁ Alkanes and alkyl residues	
3.11	A ₂ Alkenes	
3.11	A ₃ Alkynes	
3.11	A ₄ Cycloalkanes	
3.11	A ₅ Aromatic hydrocarbons	
3.11	B Halogen compounds	
3.11	C Alcohols and Phenols	
3.11	D Ethers	
3.11	E Carbonyl compounds	
3.11	E ₁ Aldehydes and ketones	
3.11	F Esters and lactones	
3.11	G Carboxylic acids	
3.11	H Acid halides	
3.11	I Acid anhydrides	
3.11	J Amides	
3.11	K Lactams	
3.11	L Amino acids	
3.11	M Amines	
3.11	N Anilides	
3.11	O Nitro and Nitrite compounds	
3.11	P Nitriles and related compounds	
3.11	Q Thiols, Sulphonic acid and Sulphonamides	



3.11	R Hetroaromatic compounds	140
3.12	Important Features in infra-red Spectroscopy	141
3.13	Applications of infra-red Spectroscopy	144
3.14	Simple Problems on infra-red Spectroscopy	147
3.15	Short questions with Answers	150
3.16	Important tips for Interpreting an infra-red Spectrum	155
3.17	Important Terms and Definitions in infra-red Spectroscopy	157
	Further Reading	158
	Review Questions	159
	Multiple Choice Questions	161

CHAPTER 4: RAMAN SPECTROSCOPY

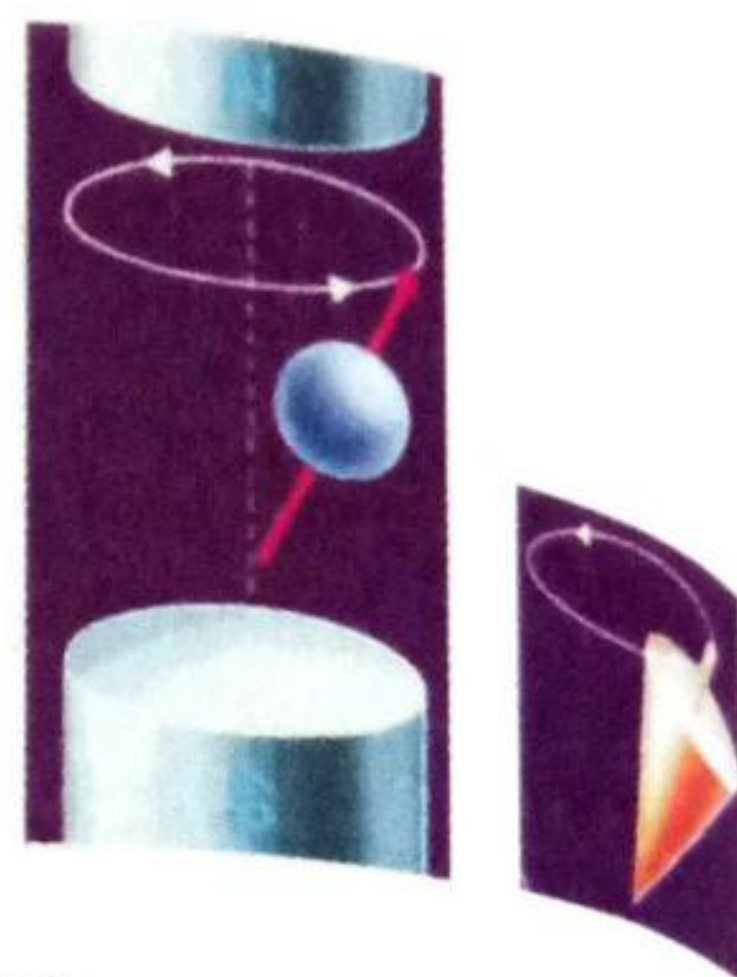
4.1	Introduction	164
4.2	Quantum Theory of Raman Effect	164
4.3	Theory of Raman Spectra (Stoke's and antistoke's lines)	164
4.4	Instrumentation	167
4.5	Conditions for Raman spectroscopy	167
4.6	Equivalence of Beer lambert law of absorption in Raman Scattering	168
4.7	Characteristic Parameters of Raman lines	168
4.8	Raman spectra of diatomic molecules	170
4.9	Rotational-Vibrational Raman Spectra	173
4.10	Vibrational Raman Spectra of Polyatomic Molecules	174
4.11	Rule of Mutual Exclusion Principle	175
4.12	Moment of Inertia of diatomic molecules, and Raman Spectroscopy	175
4.13	Infra-red and Raman Spectra are Complementary	177
4.14	Structure Elucidation by Raman Spectroscopy	178
4.15	Numericals On Raman Spectroscopy	179
4.16	Importance of Raman Spectra	181
4.17	Applications of Raman Spectroscopy	182
4.18	Important Terms and Definitions in Raman Spectroscopy	184
4.19	Short Questions with Answers	185
	Further Reading	187
	Review Questions	187
	Multiple Choice Questions	188

CHAPTER 5: NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY

5.1	Introduction	191
5.2	Relaxation Process	194
5.3	Number of Signals	195
5.4	Instrumentation	198
5.5	Positions of Signals (Chemical Shift)	198
5.6	Internal Standards	200
5.7	Shielding and Deshielding Effects*	201

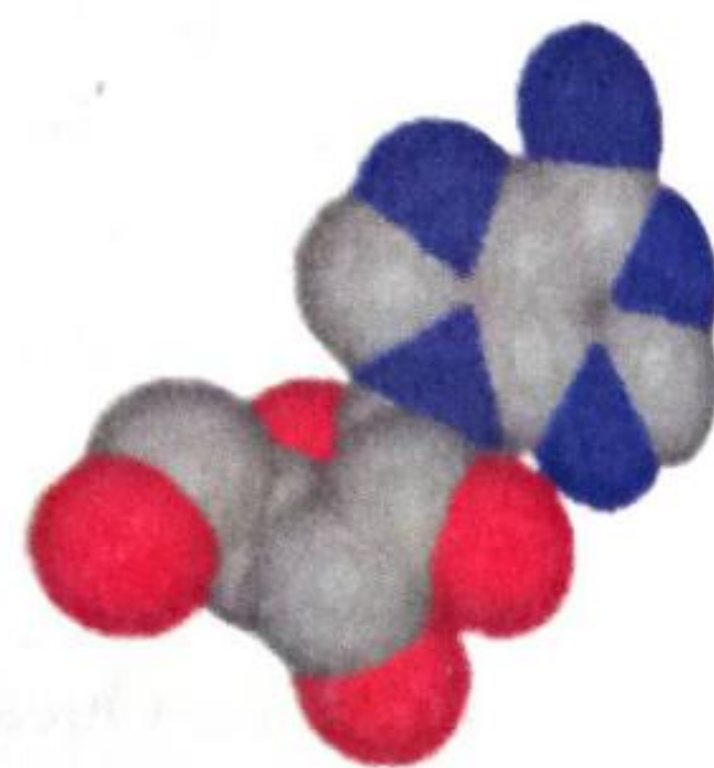


- 5.8 Factors Influencing Chemical Shift
 - 5.9 Solvents Used
 - 5.10 Peak Area and Proton Counting
 - 5.11 Splitting of the Signals
 - 5.12 Spin-spin Coupling
 - 5.13 Nmr Absorption by other Nuclei
 - 5.14 Calculating the Ratio in the heights of the Signals
 - 5.15 Chemical Exchange (Proton Exchange Reactions)
 - 5.16 Coupling Constant (J)
 - 5.17 Restricted Rotation
 - 5.18 Important Tips for Interpreting an Nmr Spectrum
 - 5.19 Some Important Nmr Spectra
 - 5.20 Double Resonance (Spin Decoupling)
 - 5.21 Nuclear Overhauser Effect (N.O.E.)
 - 5.22 Nmr Spectrum at more than one Radio-Frequency
 - 5.23 Deuterium Exchange Reactions
 - 5.24 C13-nmr Spectroscopy
 - 5.25 F19- nmr
 - 5.26 Nuclear Magnetic Resonance Spectra of Carbocations
 - 5.27 Applications of Nmr Spectroscopy
 - 5.28 Important Features in Nuclear Magnetic Resonance Spectroscopy
 - 5.29 Simple Problems on Nuclear Magnetic Resonance
 - 5.30 Short Questions with Answers
- Further Reading
Review Questions
Multiple Choice Questions



CHAPTER 6: NUMERICAL PROBLEMS ON UV; IR AND NMR

- 6.1 Double bond and/or Ring equivalents
- 6.2 Problem set with solutions
 - (Problems 1–30)
 - Problem set I (Unsolved)
 - (Problems 1–26)
 - Problem set II (Unsolved)
 - (Problems 27–50)



CHAPTER 7: MASS SPECTROMETRY

- 7.1 Basic Principles
- 7.2 Theory
- 7.3 Instrumentation
- 7.4 Mass Spectrum
- 7.5 Determination of Molecular Formula
- 7.6 McLafferty Rearrangement



7.7	Metastable Ions or Peaks	299
7.8	The Nitrogen Rule	301
7.9	General Fragmentation Modes	302
7.10	General Fragmentation Modes	305
7.10	Important Features of the Mass Spectra of Hydrocarbons	308
7.11	A Alkenes (Olefins)	308
7.11	B Acetylenes (Alkynes)	309
7.11	C Cycloalkanes	309
7.11	D Cycloalkenes and Cycloalkynes	311
7.12	Aromatic Compounds	315
7.13	Alcohols	321
7.14	Phenols	322
7.15	Thiols and Thiophenols	324
7.16	Ethers, Acetals and Ketals	326
7.17	Aliphatic Aldehydes and Ketones	329
7.18	Cyclic ketones	331
7.19	Aliphatic and Aromatic Acids	332
7.20	Esters	334
7.21	Amides	335
7.22	Halogen Compounds	337
6.23	Amines	339
6.24	Nitro Compounds	340
7.25	Aliphatic Nitriles	340
7.26	Important Features in Mass Spectroscopy	343
7.27	Simple Problems on Mass spectroscopy	345
7.27	Short Questions with Answer	350
	Further Reading	350
	Review Questions	351
	Numerical Problems on Mass Spectrometry	352
	Multiple Choice Questions	354
	Answers to Problems	357
	Subject index	364
	Compound index	

