



3.3.2

Number of books and chapters in edited volumes/books published and papers published in national/ international conference proceedings per teacher during last five years



3.3.2

A. Number of books and chapters in edited volumes/books published



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3.3. Research Publications and Awards

3.3.2 Number of books and chapters in edited volumes/books published and papers published in national/ international conference proceedings per teacher during last five year

A. Number of books and chapters in edited volumes/books published

Sr. No.	Name of the teacher	Title of the book/chapters published	National / International	Calendar Year of publication	ISBN number of the proceeding	Affiliating Institute at the time of publication	Name of the publisher
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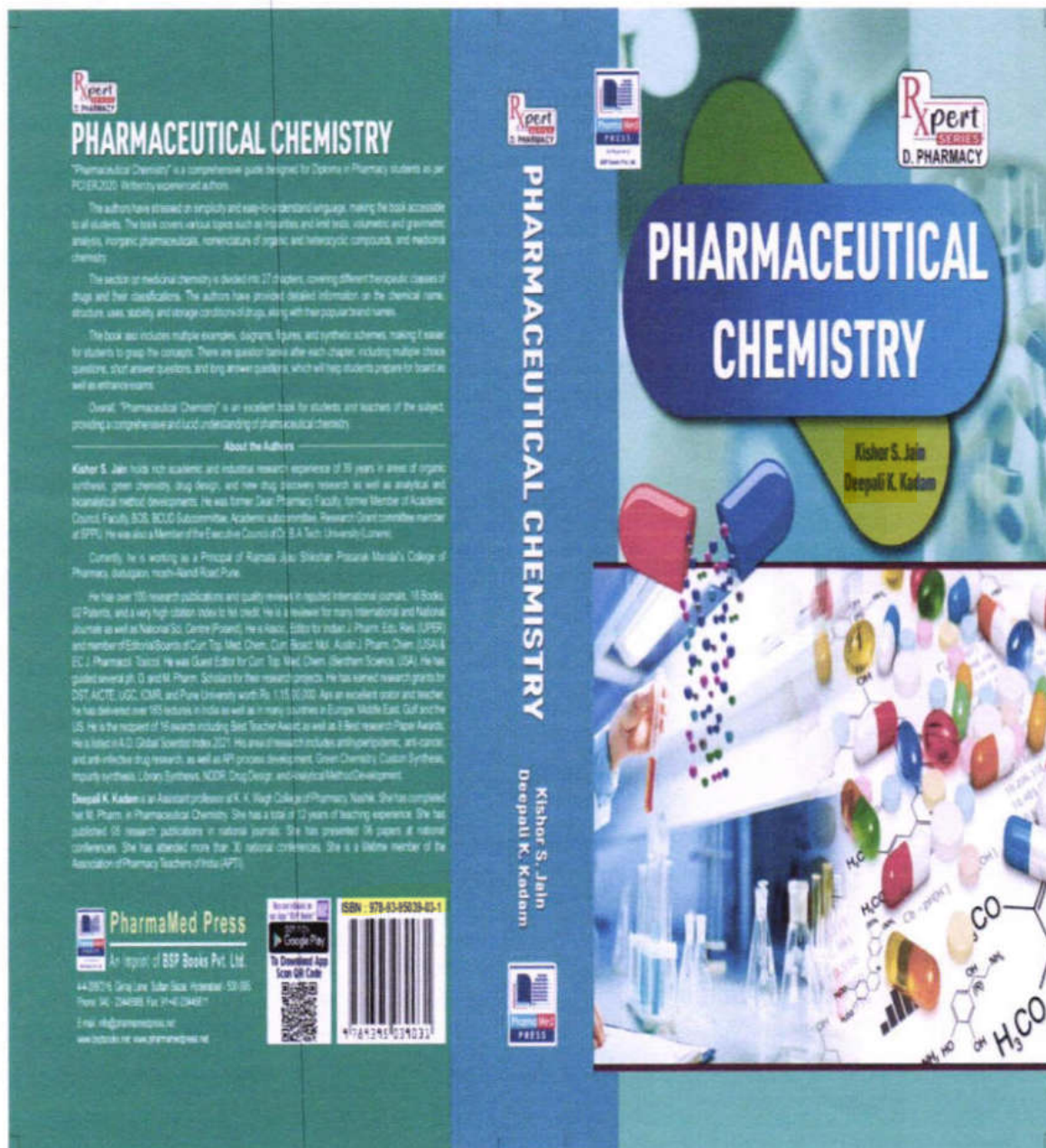



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CONTENTS

Foreword.....	(v)
Preface.....	(vii)

CHAPTER 1

Introduction to Pharmaceutical Chemistry

1.1 Introduction to pharmaceutical chemistry	1
1.2 Sources and Types of Errors, Accuracy, Precision, Significant Figures	2
1.3 Impurities in Pharmaceuticals.....	5
1.4 Limit Tests	9
Question Bank.....	21
Multiple Choice Questions	21
Short Answer Questions	23
Long Answer Questions.....	24

CHAPTER 2

Introduction to Pharmaceutical Chemistry

2.1 Fundamentals of Volumetric Analysis.....	26
2.2 Acid-base Titrations.....	35
2.3 Non-Aqueous Titrations	42
2.4 Precipitation Titration	49
2.5 Complexometric Titration.....	54
2.6 Redox Titration	59
2.7 Gravimetric Analysis: Principle and Method.....	69
Question Bank.....	75
Multiple Choice Questions.....	75
Short Answer Questions	81
Long Answer Questions	82

CHAPTER 3.1

Haematinics

3.1 Introduction.....	83
3.1.1 Haematinics	85
Question Bank.....	92

(ix)



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(x) Contents

Multiple Choice Questions.....	92
Short Answer Questions.....	93
Long Answer Questions	94

CHAPTER 3.2

Gastro-Intestinal Agents

3.2.1 Gastri-Intestinal Agents: Introduction	95
3.2.2 Acidifying Agents.....	97
3.2.3 Antacids.....	98
3.2.4 Adsorbents & Protectives	106
3.2.5 Cathartics	107
Question Bank.....	111
Multiple Choice Questions.....	111
Short Answer Questions.....	113
Long Answer Questions	114

CHAPTER 3.3

Topical Agents

3.3 Topical Agents.....	115
3.3.1 Definition:.....	115
3.3.1 Mechanism of Action.....	117
3.3.2 Commonly used Antimicrobial Agents	118
Question Bank.....	125
Multiple Choice Questions.....	125
Short Answer Questions.....	127
Long Answer Questions	127

CHAPTER 3.4

Dental Products

3.4.1 Introduction.....	128
3.4.2 Dental Products.....	130
3.4.3 MouthWash, Mouth Rinse, Oral Rinse or Mouth Bath	134
3.4.5 Preparation and Assay of Some Important Anti-Caries Agents	135
3.4.6 Dental Adhesives: Zinc Eugenol (ZOE) Dental Cement	139
Question Bank.....	140



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Multiple Choice Questions.....	140
Short Answer Questions.....	142
Long Answer Questions.....	142

CHAPTER 3.5

Medicinal Gases

3.5 Introduction.....	143
3.5.1 Carbon Dioxide.....	144
3.5.2 Nitrous Oxide.....	145
3.5.3 Oxygen.....	147
Question Bank.....	148
Multiple Choice Questions.....	148
Short Answer Questions.....	149
Long Answer Questions.....	149

CHAPTER 4

Introduction to Nomenclature

4.1 Classification of Organic Compounds.....	150
4.2 Nomenclature of Organic Compounds.....	152
4.3 Nomenclature of Heterocyclic Compounds.....	168
Question Bank.....	174
Multiple Choice Questions.....	174
Short Answer Questions.....	176
Long Answer Questions.....	177

CHAPTER 5

Drugs Acting on Central Nervous System: Anaesthetics

5. Introduction.....	179
5.1 Anaesthetics or General Anaesthetics.....	181
5.2 Classification of Anesthetics.....	185
5.3 Some Important Drugs used for General Anaesthesia.....	185
Question Bank.....	191
Multiple Choice Questions.....	191
Short Answer Questions.....	192
Long Answer Questions.....	192




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CHAPTER 5.5

Drugs Acting on the Central Nervous System: Antidepressants

5.5.1 Introduction.....	239
5.5.2 Classification of Antidepressants.....	240
5.5.3 Mechanism of Action of Antidepressants.....	240
5.5.4 Some Important Antidepressant Drugs.....	243
<i>Question Bank</i>	255
<i>Multiple Choice Questions</i>	255
<i>Short Answer Questions</i>	256
<i>Long Answer Questions</i>	256

CHAPTER 6.1

Drugs Acting on Autonomic Nervous System: Sympathomimetic Agents

6.1.1 Introduction.....	259
6.1.2 Adrenergic Receptors	261
6.1.3 Adrenergic or Sympathomimetic Agents.....	263
6.1.4 Classification of Sympathomimetic Agents as per M.O.A.....	264
6.1.5 Therapeutic Classification of Sympathomimetic Agents.....	266
6.1.6 Mechanism of Action of Sympathomimetic Agents.....	266
6.1.7 Physiological EFFECTs of Sympathomimetic Agents.....	267
6.1.8 Some Important Sympathomimetic Agents.....	268
<i>Question Bank</i>	282
<i>Multiple Choice Questions</i>	282
<i>Short Answer Questions</i>	283
<i>Long Answer Questions</i>	284

CHAPTER 6.2

Drugs Acting on Autonomic Nervous System: Adrenergic Antagonists

6.2.1 Introduction.....	285
6.2.2 Classification	286
6.2.3 Mechanism of action.....	288




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CHAPTER 5.2

**Drugs Acting on Central Nervous System:
Sedatives and Hyponotics**

5.2.1 Introduction.....	194
5.2.2 Classification of Sedatives and Hypnotics	196
5.2.3 Important Drugs used as Sedatives and Hypnotics.....	198
<i>Question Bank</i>	204
<i>Multiple Choice Questions</i>	204
<i>Short Answer Questions</i>	205
<i>Long Answer Questions</i>	206

CHAPTER 5.3

**Drugs Acting on the Central Nervous System:
Antipsychotics**

5.3.1 Introduction.....	208
5.3.2 Classification of Antipsychotic Drugs	208
5.3.3 Mechanism of Action of Antipsychotic Drugs	209
5.3.4 Some Important Drugs used as Antipsychotic Agents.....	210
<i>Question Bank</i>	219
<i>Multiple Choice Questions</i>	219
<i>Short Answer Questions</i>	220
<i>Long Answer Questions</i>	220

CHAPTER 5.4

**Drugs Acting on the Central Nervous System:
Anticonvulsants**

Introduction.....	222
5.4.1 Classification of Anticonvulsant Drugs/AEDs	224
5.4.2 Some Important Drugs used AS Anticonvulsants.....	228
<i>Question Bank</i>	236
<i>Short Answer Questions</i>	236
<i>Long Answer Questions</i>	237




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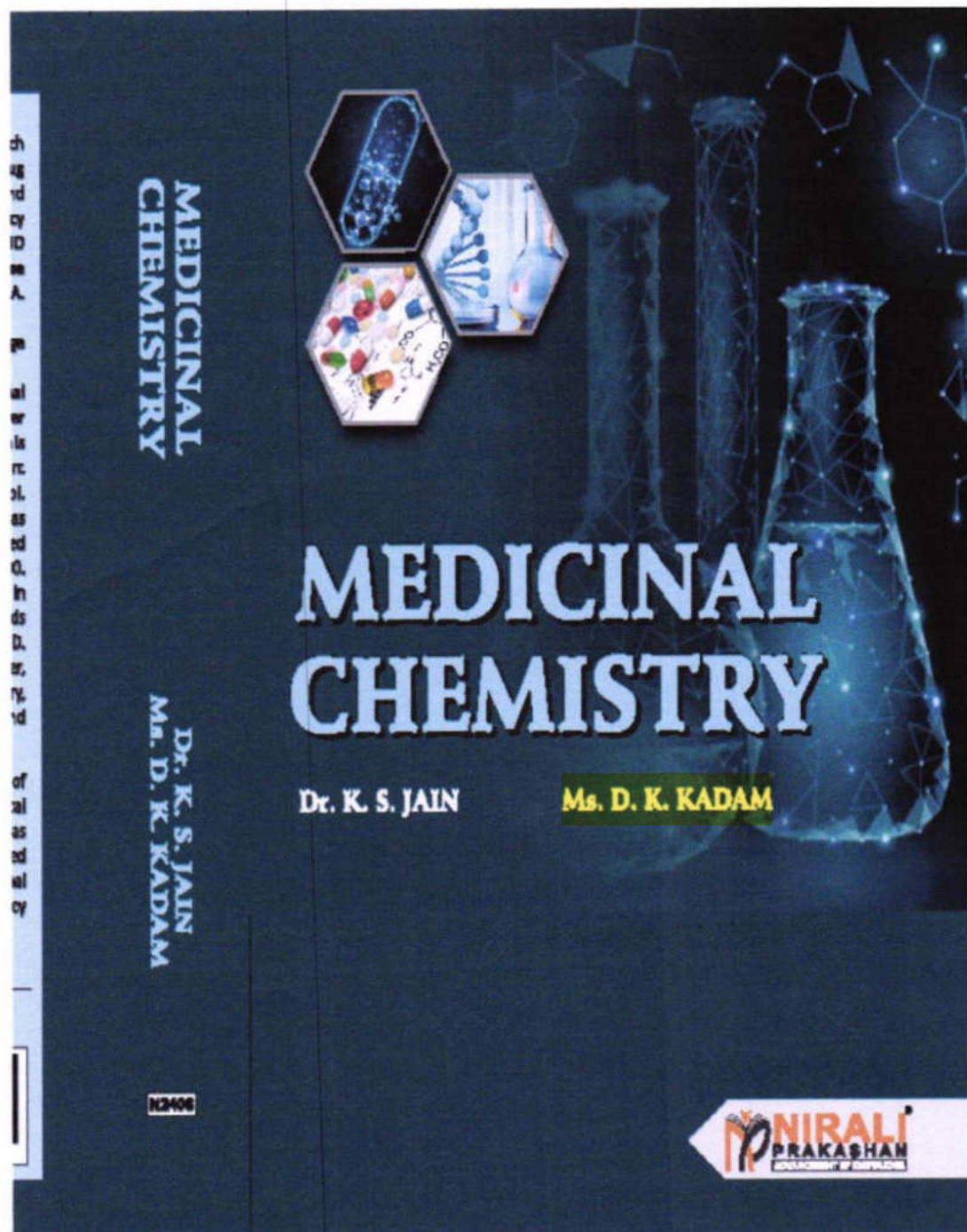



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As Per PCI Regulations

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Contents

1. History and Development of Medicinal Chemistry	1.1 – 1.16
2. Physicochemical Properties in Relation to Biological Action	2.1 – 2.31
3. Drug Metabolism	3.1 – 3.36
4. Adrenergic Neurotransmitters	4.1 – 4.36
5. Cholinergic Neurotransmitters	5.1 – 5.8
6. Parasympathomimetic Agents	6.1 – 6.17
7. Cholinergic Blocking Agents	7.1 – 7.19
8. Sedatives and Hypnotics	8.1 – 8.27
9. Antipsychotics	9.1 – 9.16
10. Anticonvulsants	10.1 – 10.29
11. General Anesthetics	11.1 – 11.24
12. Narcotic and Non-Narcotic Analgesics and Inflammatory Agents	12.1 – 12.42
13. Antihistaminic Agents and Autacoids	13.1 – 13.55
14. Anti-anginal Agents	14.1 – 14.26
15. Diuretics	15.1 – 15.21
16. Anti-hypertensive Agents	16.1 – 16.20
17. Anti-arrhythmic Drugs	17.1 – 17.29
18. Anti-hyperlipidemic Agents	18.1 – 18.21
19. Coagulants and Anticoagulants	19.1 – 19.10
20. Drugs used in Congestive Heart Failure [CHF]	20.1 – 20.8
21. Drugs Acting on Endocrine System	21.1 – 21.42
22. Thyroid and Antithyroid Drugs	22.1 – 22.10
23. Drugs for Erectile Dysfunction	23.1 – 23.7
24. Antidiabetic Agents	24.1 – 24.18
25. Local Anesthetics	25.1 – 25.22
26. Antibiotics	26.1 – 26.66




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27. Macrolide Antibiotics	27.1 - 27.12
28. Prodrugs : Basic Concepts and Application of Prodrugs Design	28.1 - 28.31
29. Antimalarials	29.1 - 29.29
30. Anti-tubercular Agents	30.1 - 30.26
31. Urinary Tract Anti-infective Agents	31.1 - 31.14
32. Antiviral Agents	32.1 - 32.20
33. Antifungal Agents	33.1 - 33.26
34. Anti-protozoal Agents	34.1 - 34.11
35. Anthelmintics	35.1 - 35.10
36. Sulfonamides and Sulfones	36.1 - 36.19
37. Anti-neoplastic Agents	37.1 - 37.30
38. Introduction to Drug Design	38.1 - 38.58




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Chapter ... 1

HISTORY AND DEVELOPMENT OF MEDICINAL CHEMISTRY

♦ LEARNING OBJECTIVES ♦

After completing this chapter, student should be able to understand:

- *Definition and Scope of Medicinal Chemistry.*
- *History and development of Medicinal Chemistry in various phases.*
- *New Drug Discovery and Development.*
- *The importance of various Physicochemical Properties of drug substances in relation to their Biological Action.*
- *The principles and phases of Drug metabolism and its importance.*
- *The Factors affecting Drug Metabolism including Stereochemical aspects and Metabolic Fate of various Drugs with selected examples.*

1.1 INTRODUCTION

1.1.1 Definition and Scope of Medicinal Chemistry

It is the branch of chemistry which deals with the fundamental knowledge on the structure, chemistry and therapeutic value of drugs. The subject emphasizes on structure activity relationships of drugs, importance of physicochemical properties and metabolism of drugs, as well as, the chemical synthesis of important drugs under each class.

Though, most of the infectious diseases like tuberculosis, typhoid, malaria, infective hepatitis, tetanus, cholera, etc., which kill lakhs of people every year in underdeveloped or developing countries, have been completely wiped off from the developed nations, some are still back in resistant forms. Also, disorders and infections like heart disease, diabetes, alzheimer, cancer and HIV infection are now considered the biggest killers.

1.1.2 The Art of Medicinal Chemistry

The science that strives to identify, create or modify molecules for therapeutic application - has enriched greatly from developments in the areas of organic chemistry, biology, biophysical/biochemical methods, and computational tools. While opportunities are enormous, advancing a drug candidate from benchtop (preclinical) to clinic (clinical) is associated with challenges. A good understanding on both these aspects would significantly accelerate drug discovery process. Really, the unprecedented increase in human life expectancy, which has almost doubled in a hundred years, is mainly due to drugs and to those who discovered them.

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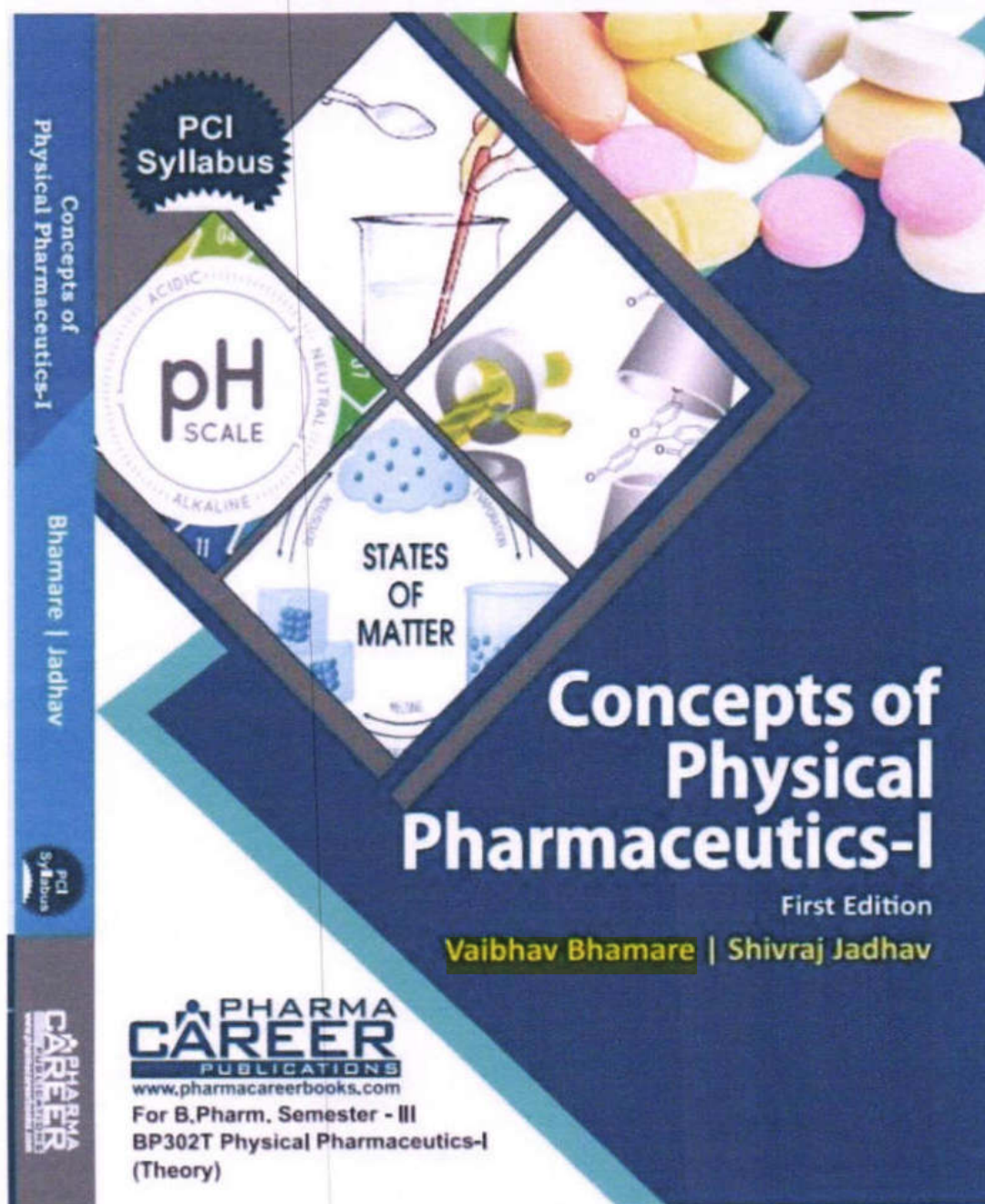



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CONTENTS

Unit	Name of Topic	Page No.
I	Solubility of Drugs	01
II	Part I - State of Matter and Properties of Matter	36
	Part II - Physicochemical Properties of Drug	73
III	Surface and Interfacial Phenomenon	91
IV	Complexation and Protein Binding	125
V	pH, Buffers and Isotonic Solution	146



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UNIT : I

SOLUBILITY OF DRUGS

Solubility expressions, Mechanisms of solute solvent interactions, Ideal solubility parameters, Solvation & Association, Factors influencing solubility of drugs, Diffusion principles in biological systems, Solubility of gas in liquids, Solubility of liquids in liquids, (Binary solutions, ideal solutions), Raoult's law, Ideal and Real solutions, Partially miscible liquids, Critical solution temperature and applications, Distribution law, its limitations and applications.

1.1 INTRODUCTION TO SOLUBILITY :

- Solubility is the important parameter to achieve desired concentration of drugs in the systemic circulation that could exert desired physiological response. Any drug to be absorbed must be present in the form of an aqueous solution at the site of absorption. Since, water remains the solvent of choice for liquid pharmaceutical formulations; poor water soluble drugs have slow absorption leading to inadequate bioavailability.
- Solubility can be defined in two ways, in quantitative way and qualitative way.
- Quantitatively solubility is defined as the maximum amount of a substance that will dissolve in a given amount of solvent at a specified temperature.
- Qualitatively solubility can be defined as spontaneous interaction between solute and solvent to form homogeneous solution.
- Generally, the solubility of a compound depends on the physical and chemical properties of the components (solute and the solvent) and several factors that have impact over process of solubilization such as temperature, pressure, pH, particle size of solute etc.
- Solubility is usually expressed as grams of solute per liter of solvent.
- A solute is any substance which can be either solid or liquid or gas dissolved in a solvent. Generally, in solution, the amount of solute is always less than solvent. For ex. Sodium Chloride, Sugar.
- A solvent is a substance that dissolves a solute. The solvent is the component of a solution that is present in higher concentration. Solvents which are generally in liquid form but can also be a solid or gas that are used to dissolve, suspend or extract other materials, usually without chemically changing either the solvents or the other materials. For ex. Water, Ethanol.



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Title of the book/chapters published- Growing impact of herbal bioenhancers in pharmaceutical industries

Name of the faculty- Dr. Vaibhav Bhamre, Dr. Rakesh Amrutkar, Mr. Vinod Patil, Dr. Chandrashekhar Upasani

Name of the publisher- De-Gruyter, Germany

Vaibhav Bhamare, Rakesh Amrutkar, Vinod Patil, Chandrashekhar Upasani

Chapter 7

Growing impact of herbal bioenhancers in pharmaceutical industries

Abstract: Ayurvedic expertise has made a significant contribution to drug research in the world, with new methods of identifying active compounds. In comparison to modern medicines, herbal medicines have succeeded to emphasize the world for their use, with advantageous therapeutic effects and fewer adverse effects. However, in vitro/in vivo findings for these herbal drugs or extracts are not so impressively correlative. Poor lipid solubility, improper molecular size, and prolonged therapy of phytoconstituents leads to poor absorption, followed by poor bioavailability and treatment expenses. Herbal bioenhancers are nontherapeutic active phytomolecules that, when co-administered at low doses, improve the bioavailability, bioefficacy, and biological activity of different drugs without having a synergistic impact with medication. Since herbal bioenhancers are healthy, nontoxic, inexpensive, easy to obtain, nonaddictive, pharmacologically inert, and nonallergenic, they are enticing pharmaceutical industries as a valuable and most effective means of bioavailability enhancement. Nowadays, industries are focusing on improvement in pharmacokinetic parameters of potent active pharmaceutical ingredients using various bioenhancing mechanisms that can help through alteration in enzyme activity, phytosomal formulation system, escape protein modifications, effects of cholagogic or choleretic agent, and heat production in the organism. An emphasis is made to tackle multidrug resistance in the treatment of infectious diseases. Bioenhancers significantly contribute to the drug development process, with innovative methods for identifying active compounds, using natural drugs and products. Herbal bioenhancers are becoming increasingly popular as a paradigm-shifting technology for improving the bioavailability and bioefficacy of various classes of drugs, nutraceuticals, and veterinary medicines, thanks to recent advances in drug delivery.

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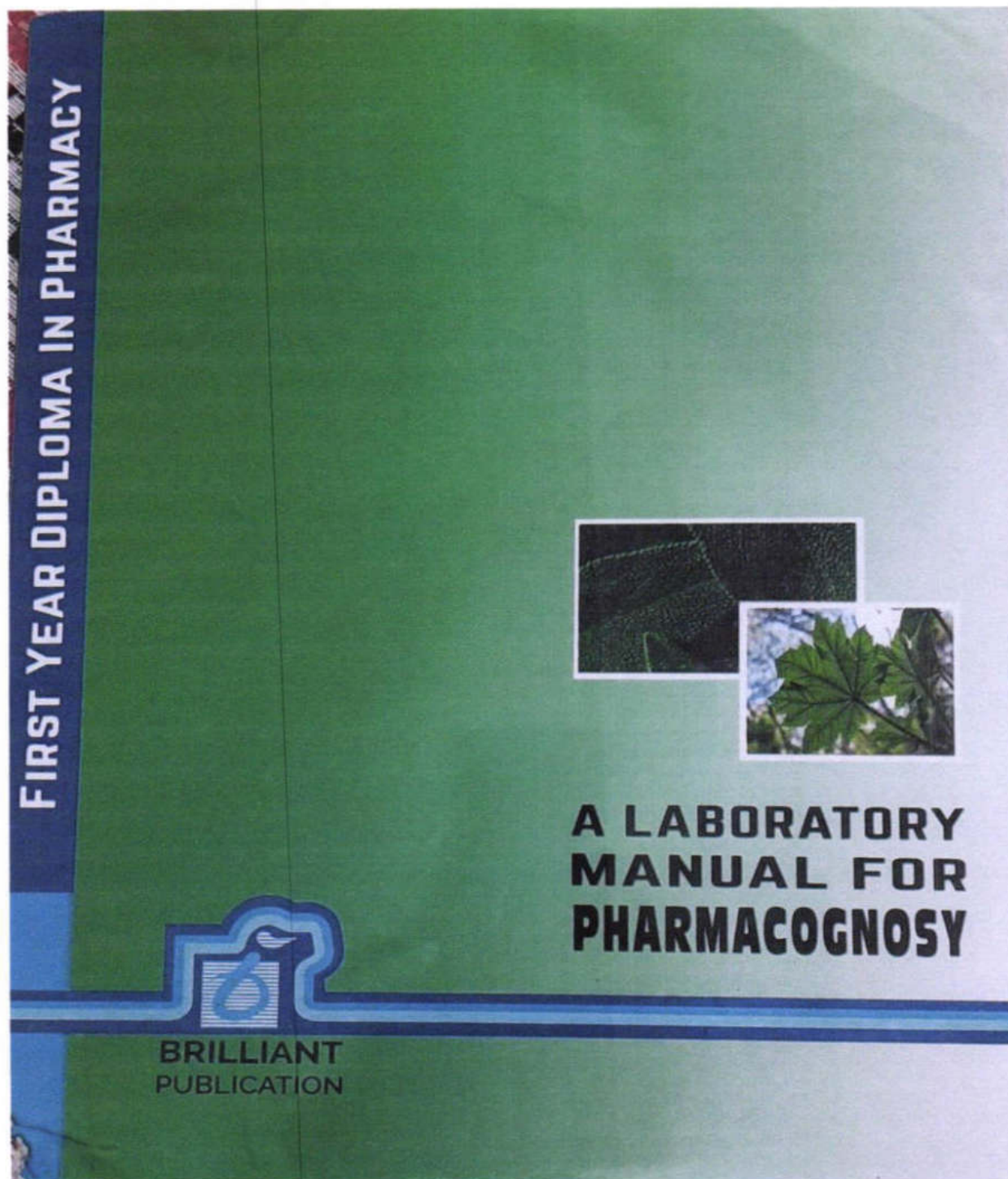


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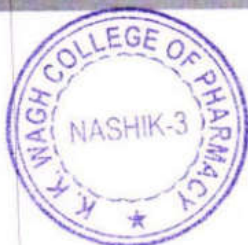
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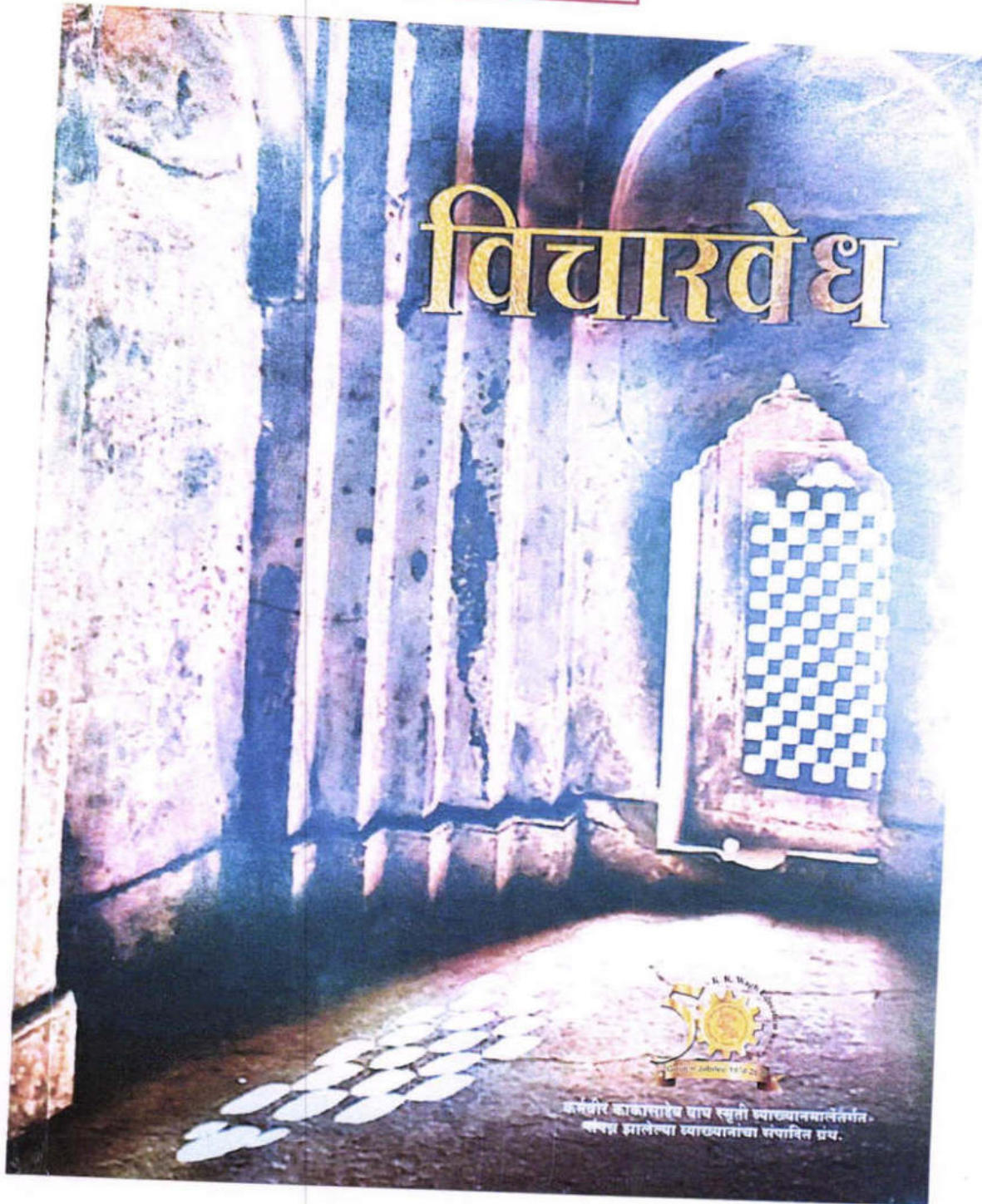
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Contents

Unit 1 : General Introduction	1.16
1.1 Volumetric Glassware	1.1
1.1.1 Pipettes	1.1
1.1.2 Burettes	1.3
1.1.3 Measuring Cylinders	1.4
1.1.4 Volumetric Flasks	1.5
1.1.5 Erlenmeyer Flasks	1.7
1.1.6 Weighing Bottles and Specific Gravity Bottles	1.8
1.1.7 Beakers	1.9
1.2 Cleaning of Glassware	1.9
1.3 Some Basic Concepts	1.9
1.3.1 Preparation of Aqueous Solutions	1.9
1.3.2 Per cent Solutions	1.11
1.4 Volumetric Methods	1.11
1.4.1 Definitions of Terms	1.11
1.4.2 Requirements for Volumetric Methods	1.12
1.4.3 Classification of Volumetric Methods	1.12
1.4.4 Steps Involved in Quantitative Analysis	1.13
1.4.5 End Point Detection	1.14
1.4.6 Calibration of Volumetric Glasswares	1.15
• Question Bank for Viva-Voce	1.16
 Unit 2 : Limits Tests	 2.1 - 2.20
Experiment 1 : To Perform Limit Test for Chlorides	2.3
Experiment 2 : To Perform Limit Test for Sulphate	2.6
Experiment 3 : To Perform Limit Test for Iron	2.9
Experiment 4 : To Perform Limit Test for Arsenic	2.11
• Question Bank for Viva-Voce	2.17
 Unit 3 Preparation and Standardization of Some Volumetric Reagent Solutions	 3.1 - 3.14
Experiment 1 : To Prepare and Standardize 0.1 N Sodium Hydroxide	3.1
Experiment 2 : To Prepare and Standardize 0.5 M Sulphuric Acid	3.3
Experiment 3 : To Prepare and Standardize 0.1 N Sodium Thiosulfate	3.4
Experiment 4 : To Prepare and Standardize 0.1 N Potassium Permanganate	3.6
Experiment 5 : To Prepare and Standardize 0.1 M Ceric Ammonium Sulphate	3.10
• Question Bank for Viva-Voce	3.11



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Unit 4 : Assay of the Compounds Along with Standardization of Titrant 4.1 - 4.14

- Experiment 1 :** Assay of Ammonium Chloride by Acid-Base Titration 4.1
Experiment 2 : Assay of Ferrous Sulphate by Cerimetry 4.2
Experiment 3 : Assay of Copper Sulphate by Iodometry 4.3
Experiment 4 : Assay of Calcium Gluconate by Complexometry 4.5
Experiment 5 : Assay of Hydrogen Peroxide by Permanganometry 4.7
Experiment 6 : Assay of Sodium Benzoate by Non-Aqueous Titration 4.9
Experiment 7 : Assay of Sodium Chloride by Precipitation Titration 4.10
• Question Bank for Viva-Voce 4.12

Unit 5 : Determination of Normality by Electro-Analytical Methods 5.1 - 5.10

- 1. Conductometric Titrations 5.1**
Experiment 1 : Determination of the Strength of a Solution of Strong Acid (Hydrochloric Acid) by A Standard Solution of Strong Base (Sodium Hydroxide) 5.1
Experiment 2 : To Carry Out the Conductometric Titration of Mixture of Acids [0.1N HCl + 0.1N CH₃COOH] vs. Strong Base (1 N NaOH) 5.5
2. Potentiometric Titrations 5.7
Experiment 3 : Determination of Strength of Strong Acid Against Strong Base by Potentiometric Titration 5.7
• Question Bank for Viva-Voce 5.9

Bibliography

B.1 - B.1

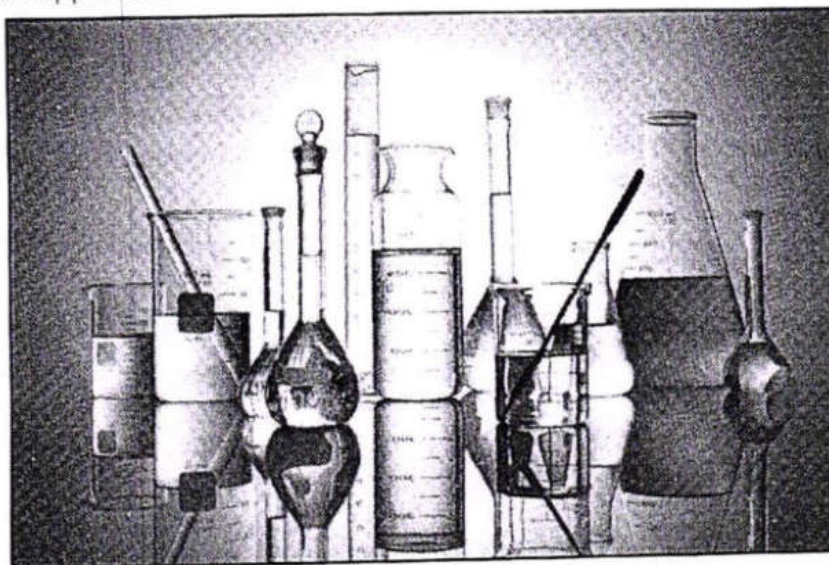



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Unit...1

GENERAL INTRODUCTION

All laboratory work involves some form of measurement. Various types of volumetric glassware are available for measuring lab reagents. Before starting any analytical experiment, one must familiarize him/herself with the types of volumetric glassware and should learn to use the apparatus accurately to eliminate the errors resulting from careless handling of the apparatus.



1.1 VOLUMETRIC GLASSWARE

1.1.1 Pipettes

These are used to transfer a known volume of liquid from one container to another. They are designed either to contain (TC) a specific volume of liquid or to deliver (TD) a specified volume. [To contain and To deliver (TC & TD): Manufacturer stamp TC or TD near the top of the pipette. TC pipette holds or contains a particular volume but does not dispense that exact volume, whereas TD pipette will dispense the exact volume indicated].

Table 1.1 : Pipette Classification

- | |
|--------------------|
| I. Design |
| A. To contain (TC) |
| B. To deliver (TD) |

(1.1)



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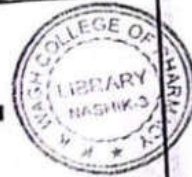
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Contents

Unit I : Introduction to Pharmaceutical Analysis

1. Pharmaceutical Analysis	1.1 - 1.18
✓ 1.1 Introduction: Definition & Scope of Pharmaceutical Analysis	1.1
1.2 Different Techniques of Analysis	1.2
1.3 Methods of Expressing Concentration	1.4
1.4 Primary and Secondary Standards	1.6
1.4.1 Primary Standards	1.6
1.4.2 Secondary Standards	1.8
1.5 Preparation and Standardization of Various Molar and Normal Solutions: Oxalic Acid, Sodium Hydroxide, Hydrochloric Acid, Sodium Thiosulphate, Sulphuric Acid, Potassium Permanganate and Ceric Ammonium Sulphate	1.9
1.5.1 Preparation of Standard Solutions	1.9
1.5.1.1 Preparation of N/10 H_2SO_4	1.11
1.5.1.2 Preparation of N/10 Na_2CO_3 Solution	1.11
1.5.1.3 Preparation of N/10 NaOH Solution	1.12
1.5.1.4 Preparation of N/10 Oxalic Acid	1.12
1.5.1.5 Preparation of N/10 $KMnO_4$ Solution	1.12
1.5.1.6 Preparation of 0.1 N Hydrochloric Acid	1.13
1.5.1.7 Sodium Thiosulfate, (0.1 N) $Na_2S_2O_3 \cdot 5H_2O$ (248.19)	1.14
1.5.1.8 Ceric Ammonium Sulfate, (0.1 M) $(NH_4)_4Ce(SO_4)_4 \cdot 2H_2O$	1.15
• Question Bank	1.16
2. Errors in Chemical Analysis	2.1 - 2.10
✓ 2.1 Introduction	2.1
2.2 Precision	2.2
✓ 2.3 Accuracy	2.3
2.4 Significant Figures	2.3
2.5 Sources of Errors in Experimental Chemical Analysis	2.4
✓ 2.6 Types of Errors	2.4
2.7 Methods of Minimizing Errors	2.7
2.8 Methods to Minimize and Detect Determinate Errors	2.7
• Question Bank	2.8
3. Pharmacopoeia, Sources of Impurities, Limit Tests	3.1 - 3.40
3.1 Pharmacopoeia	3.1
3.1.1 Indian Pharmacopoeia	3.1
3.1.2 British Pharmacopoeia	3.4
3.1.3 European Pharmacopoeia	3.6



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3.1.4	United States Pharmacopoeia (USP)	3.7
3.1.5	Pharmacopoeia International (International Pharmacopoeia)	3.8
3.1.6	Extrapharmacopoeia (Martindale)	3.9
3.2	Sources of Impurities in Pharmaceuticals	3.10
3.2.1	Sources and Effects of Impurities in Pharmacopoeial Substances	3.10
3.2.2	Effects of Impurities on Pharmaceuticals	3.13
3.3	Limit Tests	3.13
3.3.1	Importance of Limit Tests	3.13
3.3.2	Principle and Procedure of Limit Test for Chloride	3.15
3.3.2.1	Principle and Procedure of Modified Limit Test for Chloride	3.16
3.3.2.2	Principle and Procedure of Limit Test for Sulphate	3.17
3.3.2.3	Principle and Procedure of Limit Test for Sulphate	3.19
3.3.2.4	Principle and Procedure of Limit Test for Iron	3.20
3.3.2.5	Principle and Procedure of Limit Test for Lead	3.22
3.3.2.6	Principle and Procedure of Limit Test for Arsenic	3.27
3.3.2.7	Principle and Modified Procedure of Limit Test for Arsenic for Different Compounds	3.30
3.3.2.8	Principle and Procedure of Limit Test for Heavy Metals	3.33
•	Question Bank	3.37

Unit II

4. Acid Base Titrations	4.1 – 4.20
4.1 Concepts of Acid and Base	4.1
4.1.1 Arrhenius Theory	4.1
4.1.2 Lowry and Bronsted's Theory	4.1
4.1.3 Lewis's Theory	4.3
4.1.4 Usanovich Theory	4.3
4.1.5 Lux-Flood Concept	4.4
4.2 Theories of Acid-Base Indicators	4.4
4.2.1 Indicator Range	4.5
4.2.2 Ostwald's Theory	4.5
4.2.3 Quinonoid Theory	4.7
4.3 Theory Involved in Titrations of Strong, Weak and Very Weak Acids and Bases	4.8
4.4 Buffer Equations and Buffer Capacity	4.8
4.5 Neutralization Curves	4.11
4.5.1 Neutralization Curve for Strong Acid and Strong Base Titration	4.11
4.5.2 Neutralization Curve for Weak Acid and Strong Base Titration	4.13
4.5.3 Titration Curve between Weak Base and Strong Acid Titration	4.15
4.5.4 Titration Curve between Weak Acid and Weak Base	4.17
• Question Bank	4.19





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5. Non-Aqueous Titrations

5.1 - 5.14

5.1	Introduction	5.1
5.2	Advantages of Non-aqueous Titrations	5.1
5.3	Solvents used in Non-aqueous Titration	5.2
5.3.1	Properties of Non-aqueous Solvent	5.2
5.3.2	Different Types of Solvents	5.2
5.4	Levelling Effect, Leveling and Differentiating Solvents	5.4
5.5	Methodology for Non-aqueous Titrations	5.4
5.5.1	Preparation of 0.1 N Perchloric Acid	5.4
5.5.2	Standardization of 0.1 N Perchloric Acid	5.5
5.5.3	Choice of Indicators	5.6
5.5.4	Effect of Temperature on Assays	5.6
5.6	Assays by Non-aqueous Titrations	5.7
5.6.1	Acidimetry in Non-aqueous Titrations	5.7
5.6.1.1	Titration of Primary, Secondary and Tertiary Amines	5.7
5.6.1.2	Titration of Halogen Acid Salts of Bases	5.8
5.6.1.2.1	Amitriptyline Hydrochloride	5.8
5.6.2	Alkalimetry in Non-Aqueous Titrations	5.8
5.6.2.1	Preparation of 0.1 N Potassium Methoxide in Toluene-Methanol	5.9
5.6.2.2	Preparation of 0.1 N Sodium Methoxide	5.9
5.6.2.3	Preparation of 0.1 N Lithium Methoxide	5.9
5.6.2.4	Standardization of 0.1 N Methoxide Solution	5.9
5.7	Estimation of Sodium Benzoate and Ephedrine HCl	5.10
5.8	Applications of Non-aqueous Titration	5.11
•	Question Bank	5.12

Unit III

6. Precipitation Titrations

6.1 - 6.12

6.1	Introduction	6.1
6.2	Solution Process	6.1
6.3	Factors Affecting Solubility	6.2
6.4	Detection of End Point	6.5
6.4.1	Mohr's Method	6.5
6.4.2	Volhard's Method	6.6
6.4.3	Fajan's Method	6.7
6.5	Estimation of Sodium Chloride	6.9
6.6	Classification of Methods in Precipitation Titration	6.9
6.7	Applications of Precipitation Titrations	6.10
•	Question Bank	6.10



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7. Complexometric Titrations	7.1 - 7.16
7.1 Introduction and Definition	7.1
7.2 Ligands (Complexing Agent)	7.2
7.2.1 Classification of Ligands	7.2
7.2.2 Chelating Agents	7.2
7.2.3 EDTA	7.3
7.3 Stability Constant	7.4
7.3.1 Factors Affecting Stability Constant	7.5
7.3.1.1 Effect of pH	7.5
7.3.1.2 Thermodynamic/Chelon Effect	7.6
7.3.1.3 Macrocyclic Effect	7.6
7.3.1.4 Effect of Temperature	7.6
7.3.1.5 Addition of Electrolytes	7.6
7.4 Detection of End Point	7.7
7.4.1 Visual Indicators	7.7
7.4.1.1 Metallochromic Indicators	7.7
7.4.1.2 pH Indicators	7.10
7.4.2 Instrumental Methods	7.10
7.4.2.1 Potentiometric Method	7.10
7.4.2.2 Spectrophotometric Method	7.10
7.4.2.3 Amperometric Method	7.10
7.5 Types of Titration	7.10
7.5.1 Direct Titrations	7.10
7.5.2 Back Titration	7.11
7.5.3 Replacement Titration/ Displacement Titration	7.11
7.5.4 Indirect Titration	7.11
7.5.5 Alkalimetric Titration	7.12
7.6 Titration of Mixtures	7.12
7.7 Applications of Complexometric Titrations	7.13
7.8 Estimation of Magnesium Sulphate	7.14
7.9 Estimation of Calcium Gluconate	7.14
• Question Bank	7.15
8. Gravimetry	8.1 - 8.18
8.1 Introduction	8.1
8.2 Types of Precipitates	8.2
8.2.1 Crystalline Precipitates	8.2
8.2.2 Colloidal Precipitates	8.3
8.2.2.1 Types of Colloidal Precipitates	8.4
8.2.2.2 Peptization of Colloids	8.4
8.2.3 Gelatinous Precipitates	8.5



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8.3	Precipitation Process and Particle Size	8.5
8.4	Digestion of Precipitates (Ostwald Ripening)	8.6
8.5	Purity of Precipitates	8.6
8.5.1	Co-precipitation	8.6
8.5.1.1	Surface Adsorption	8.7
8.5.1.2	Mixed Crystal Formation	8.7
8.5.1.3	Occlusion and Mechanical Entrapment	8.7
8.5.2	Post Precipitation	8.8
8.6	Precipitation from Homogenous Solution	8.8
8.7	Precipitating Agents	8.9
8.7.1	Inorganic Precipitants	8.9
8.7.2	Reducing Agents	8.9
8.7.3	Organic Precipitants	8.9
8.7.3.1	Advantages of Organic Precipitants	8.11
8.7.3.2	Disadvantages of Organic Precipitants	8.11
8.8	Advantages of Gravimetric Methods	8.11
8.9	Unit Operations in Gravimetric Analysis	8.11
8.10	Estimation of Barium Sulphate	8.15
8.10.1	Principle	8.15
8.10.2	Procedure	8.15
	• Question Bank	8.16
9.	Diazotization Titration (Sodium Nitrite Titration)	9.1 – 9.6
9.1	Introduction	9.1
9.2	Theory	9.1
9.3	Condition for Diazotization	9.2
9.3.1	Rate of Titration	9.2
9.3.2	Temperature	9.2
9.4	Principle	9.2
9.5	Types of Diazotization Titrations	9.3
9.5.1	Direct Titrations	9.3
9.5.2	Reverse Method	9.3
9.5.3	Special Method	9.3
9.6	Preparation and Standardization of 1 M Sodium Nitrate	9.3
9.6.1	Preparation of 1M Sodium Nitrate	9.3
9.6.2	Standardization of 1M Sodium Nitrate with Sulphanilamide	9.3
9.7	Assay of Calcium Aminosaliclate	9.4
9.8	Applications of Diazotization Titration	9.5
	• Question Bank	9.5



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Unit IV

10. Redox Titrations

10.1 - 10.16

10.1	Introduction	10.1
10.2	Concepts of Oxidation and Reduction	10.1
10.3	Balancing of Half Reactions	10.2
10.4	Equivalent Weights	10.4
10.5	Redox Potential	10.4
10.6	Detection of End Point in Redox Titrations	10.5
10.6.1	Internal Indicators	10.5
10.6.2	Self Indicators	10.6
10.6.3	External Indicators	10.6
10.6.4	Specific Indicators	10.6
10.6.5	Potentiometric Method	10.6
10.7	Redox Titrations	10.7
10.7.1	Titration using Potassium Permanganate	10.7
10.7.2	Cerimetry	10.8
10.7.3	Iodine Titrations	10.9
10.7.4	Bromatometry	10.13
10.7.5	Dichrometry	10.14
10.7.6	Titration with Potassium Iodate	10.15
	• Question Bank	10.15

Unit V : Electrochemical Methods of Analysis

11. Conductometry

11.1 - 11.13

11.1	Introduction	11.1
11.2	Measurement of Conductivity	11.4
11.3	Conductometric Titrations	11.7
11.3.1	Acid-Base Titrations	11.7
11.3.1.1	Strong Acid with a Strong Base	11.8
11.3.1.2	Strong Acid with Weak Base	11.8
11.3.1.3	Weak Acid with a Strong Base	11.9
11.3.1.4	Weak Acid with Weak Base	11.9
11.3.2	Precipitation Titrations	11.10
11.3.3	Redox Titrations	11.10
11.3.4	Complexometric Titrations	11.11
11.3.5	Non-aqueous Titrations	11.11
11.4	Applications	11.12
	• Question Bank	11.12



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12. Potentiometry	12.1 - 12.14
12.1 Introduction	12.1
12.2 Electrode Potential	12.1
12.3 Cell	12.2
12.3.1 Galvanic Cell	12.2
12.4 Electrodes	12.4
12.4.1 Reference Electrodes	12.4
12.4.1.1 The Standard Hydrogen Electrode (SHE)	12.4
12.4.1.2 Calomel Electrode	12.6
12.4.1.3 Silver Chloride Electrode	12.7
12.4.2 Indicator Electrodes	12.8
12.4.2.1 Metal Electrode	12.8
12.4.2.2 Glass Electrode	12.8
12.5 Methods to Determine End Points	12.10
12.6 Types of Potentiometric Titrations	12.11
12.7 Applications of Potentiometric Titrations	12.12
• Question Bank	12.13
13. Polarography	13.1 - 13.14
13.1 Introduction	13.1
13.2 Principle	13.1
13.3 Theory of Polarography	13.2
13.3.1 Polarization of Electrodes	13.2
13.4 Construction and Working of Dropping Mercury Electrode and Rotating Platinum Electrode	13.3
13.4.1 Dropping Mercury Electrode	13.3
13.4.2 Rotating Platinum Electrode	13.8
13.4.3 Polarographic Modes	13.9
13.5 Applications	13.11
• Question Bank	13.13
Index	I.1 - I.2
Bibliography	B.1 - B.1



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Unit I : Introduction to Pharmaceutical Analysis

Chapter 1

PHARMACEUTICAL ANALYSIS

♦ LEARNING OBJECTIVES ♦

After completing this chapter, student should be able to understand:

- Definition and scope of Pharmaceutical analysis.
- Various analytical techniques.
- Methods of expressing concentration.
- Standard solutions used in analysis.
- Preparation of solutions of various concentrations.

1.1 INTRODUCTION: DEFINITION & SCOPE OF PHARMACEUTICAL ANALYSIS

Definition:

Pharmaceutical analysis is a branch of practical chemistry that involves a series of processes for identification, determination, quantification and purification of a substance, separation of the components of a solution or mixture, or determination of structure of chemical compounds. The substance may be a single compound or a mixture of compounds and it may be isolated or in any of the dosage forms. The substances used as pharmaceuticals are from various synthetic or natural (animal, plant, marine, microbial or mineral) sources.

Scope:

The process of analysis can be broadly categorized as; a) qualitative (identification) and b) quantitative (estimation). The sample to be analysed is called as **analyte** and on the basis of size of analyte, quantitative analysis can be termed as; macro (0.1 gm or more), semi-micro (0.01 gm to 0.1 gm), micro (0.001 gm to 0.01 gm), sub-micro (0.0001 gm to 0.001 gm), ultra-micro (below 10^{-4} gm) and trace analysis (100 to 10000 ppm).

1. **Qualitative analysis** is performed to establish composition of natural/synthetic substances. These tests are performed to indicate whether the substance or compound is present in the sample or not. Various qualitative tests involve; detection of evolved gas, formation of precipitates, limit tests, colour change reactions, determination of melting point and boiling point etc.
2. **Quantitative analysis** is mainly used to quantify any compound or substance in the sample. These techniques are based on (a) the quantitative performance of suitable chemical reaction and either measuring the amount of reagent added to complete

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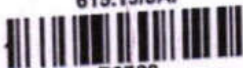
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Contents

1. Systematic Qualitative Analysis of Unknown Organic Compounds

- | | |
|--|------------|
| 1. Preliminary Tests | 1.1 - 1.82 |
| 2. Elemental Analysis or Lassaigne's Test | 1.6 |
| 3. Compounds: Elements wise and Functional groupwise | 1.17 |
| 4. Preparation of Derivatives | 1.21 |
| 5. Physical Constants and Derivatives | 1.54 |
| 6. Separation of Binary Mixture | 1.67 |
| | 1.78 |

2. Building Molecular Models of Simple Covalent Molecules

2.1 - 2.8

3. Laboratory Techniques

3.1 - 3.11

4. Analysis of Oils

4.1 - 4.7

- | | |
|--|-----|
| Experiment 1 : Determination of Acid Value | 4.2 |
| Experiment 2 : Determination of Saponification Value | 4.3 |
| Experiment 3 : Determination of Ester Value | 4.4 |
| Experiment 4 : Determination of Peroxide Value | 4.4 |
| Experiment 5 : Determination of Iodine Value | 4.5 |

5. Preparation of Compounds

5.1 - 5.30

- | | |
|---|------|
| Experiment 1 : Synthesis of Benzanilide from Aniline | 5.1 |
| Experiment 2 : Synthesis of 2 Naphthyl Benzoate from β -Naphthol | 5.2 |
| Experiment 3 : Synthesis of Phenyl Benzoate from Phenol | 5.4 |
| Experiment 4 : Synthesis of Acetanilide from Aniline | 5.6 |
| Experiment 5 : Synthesis of p-nitroacetanilide from Acetanilide | 5.8 |
| Experiment 6 : Synthesis of 2, 4, 6-tribromoaniline from Aniline | 5.11 |
| Experiment 7 : Synthesis of p-bromoacetanilide from Acetanilide | 5.13 |
| Experiment 8 : Synthesis of m-dinitrobenzene from Nitrobenzene | 5.16 |
| Experiment 9 : Synthesis of Nitrobenzene by Nitration Reaction | 5.18 |
| Experiment 10 : Synthesis of Benzoic acid from Benzyl chloride by Oxidation Reaction | 5.20 |
| Experiment 11 : Synthesis of Benzoic Acid from ethyl Benzoate by base Hydrolysis | 5.20 |
| Experiment 12 : Synthesis of Salicylic Acid from Alkyl Salicylate by Hydrolysis Reactions | 5.22 |
| Experiment 13 : Synthesis of Benzil from Benzoin | 5.24 |
| Experiment 14 : Synthesis of Phenylazo-2-naphthol from Aniline by Diazotisation Coupling reaction | 5.25 |
| Experiment 15 : Synthesis of Dibenzalacetone from Benzaldehyde | 5.26 |
| Experiment 16 : Synthesis of Cinnamic Acid from Benzaldehyde | 5.28 |

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Chapter 1 ...

Systematic Qualitative Analysis of Unknown Organic Compounds

Qualitative organic analysis is the systematic identification and confirmation of an unknown organic compound.

Qualitative organic analysis forms an important part of the practical training of the budding organic chemist. It gives a balance between structured systemic approach and the intuition, which the student acquires with experience.

Proper application of knowledge of organic chemistry and significant observations can help draw meaningful conclusions leading to pinpoint identification.

The systematic steps of qualitative analysis:

Following essential and integral steps for the systematic identification of an unknown organic compound, should be followed meticulously and religiously, skipping none of it.

1. **Preliminary tests:** It can tell the state, nature and type in a broad manner.
2. **Detection of elements/elemental analysis (Lassaigne's test):** It can throw light on which of the elements N, [O], S, halogens are present.
3. **Detection of functional group:** Which is the main organic functional group in the compound.
4. **Derivative preparation:** This is preparable and can help to confirm the unknown compound.
5. **Determination of physical constants:** B.P. or M.P. are an important characteristic physical property.
6. **Separation of binary mixture:** In case of mixture of two unknown compounds, which need to be separated prior to their analysis.

This helps in error free identification of an unknown organic compound. The tests are given in sequence one after the other, to reach the end results and to confirm the identity of the given, unknown organic compound, correctly and student is required to follow the same sequence.

Main class of organic compounds encountered in the systematic qualitative analysis:

(a) **Carbohydrates:** (e.g., glucose, fructose, sucrose, lactose, maltose, starch, dextrin, etc.)

Tests:

1. **Molisch test:** General test for carbohydrates.
2. **Barfoed's test:** For distinction between mono and disaccharides.
3. **Fehling's and Benedict's tests:** For differentiating between a reducing and a non-reducing saccharides.
4. **Selvinoff's test:** Test for ketoses.

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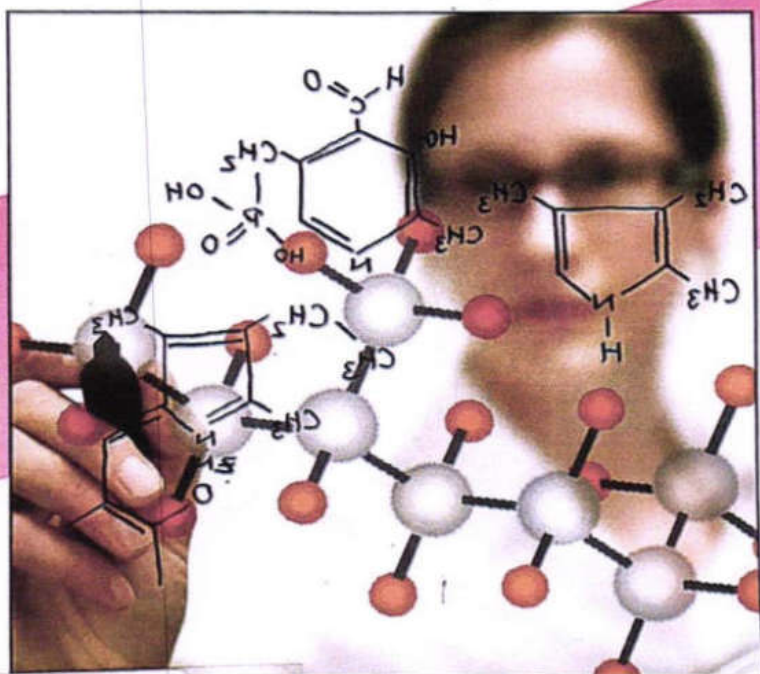
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Contents

Unit I

1. Classification, Nomenclature and Isomerism	1.1 – 1.37
1.1 Classification of Organic Compounds	1.1
1.2 Common names of Organic Compounds	1.4
1.2.1 Compounds containing Carbon and Hydrogen Only	1.4
1.2.2 Compounds containing Carbon, Hydrogen and Oxygen	1.6
1.2.3 Compounds containing Carbon, Hydrogen and Nitrogen only	1.9
1.2.4 Compounds containing Carbon, Hydrogen, Oxygen and Halogens only	1.10
1.2.5 Compounds containing Carbon, Hydrogen, Oxygen, Nitrogen and Halogens only	1.11
1.2.6 Compounds containing Carbon, Hydrogen, Oxygen, Nitrogen, Sulphur and/or Halogens	1.13
1.3 IUPAC Nomenclature System for Organic Compounds: General Rules	1.15
1.4 Isomerism	1.27
1.4.1 Constitutional or Structural Isomerism	1.27
1.4.2 Stereoisomerism	1.32
• Questions	1.34

Unit II

2. Alkanes	2.1 – 2.8
2.1 Introduction	2.1
2.2 Hybridization of Atomic Orbitals	2.3
2.3 Halogenation of Alkanes	2.5
2.4 Uses of Paraffins (alkanes)	2.7
• Questions	2.8
3. Alkenes	3.1 – 3.18
3.1 Introduction: Properties of Alkenes	3.1
3.2 Elimination Reactions-Type	3.4
3.2.1 The Mechanisms of Elimination Reaction (β -Elimination)	3.5
3.2.2 Orientation of Elimination	3.7
3.2.3 Comparison of E_1 , E_2 and E_{1cB} Reactions	3.12
3.2.4 Ozonolysis	3.13
3.3 Addition Reactions of Alkenes: Electrophilic Additions	3.14
3.4 The Markovnikoff's Orientation in Electrophilic Addition	3.17
• Questions	3.18
4. Conjugated Dienes	4.1 – 4.9
4.1 Introduction	4.1
4.2 Stability of Conjugated Dienes	4.2
4.3 Diel's-Alder Reaction	4.4
4.4 Electrophilic Addition Reaction	4.5
4.5 Free Radical Addition Reactions	4.7
4.6 Allylic Rearrangement	4.8
• Questions	4.9



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K K Wagh College of Pharmacy
Nashik-422 003

Unit III

5. Alkyl Halides

5.1	Introduction	5.1 – 5.24
5.2	General Reactions of Alkyl Halides	5.1
5.3	Factors affecting SN_1 and SN_2 Reaction Mechanisms	5.4
5.4	Substitution Vs Elimination	5.11
5.5	Structures and Uses of Some Alkyl halide derivatives	5.14
	• Questions	5.17
		5.23

6. Alcohols

6.1	Introduction	6.1 – 6.10
6.2	Nomenclature	6.1
6.3	Physical Properties	6.2
6.4	Qualitative Tests	6.3
6.5	Structure and Uses of some Alcohols	6.4
	• Questions	6.6
		6.10

Unit IV

7. Carbonyl Compounds

7.1	Nucleophilic Addition	7.1 – 7.28
7.1.1	Mechanism of Nucleophilic Addition and Condensation Reactions	7.1
7.1.2	Examples of Nucleophilic Addition to Carbonyl Groups	7.1
7.1.3	Acetal-Preparation and Uses / Addition of Alcohols to $C=O$	7.2
7.1.4	Additions of Derivatives of Ammonia	7.4
7.2	Electromeric Effect	7.6
7.3	Some Reactions of Carbonyl Compounds	7.12
7.3.1	Aldol Condensation	7.13
7.3.2	Crossed Aldol Condensation	7.13
7.3.3	Cannizaro Reaction	7.14
7.3.4	Crossed Cannizaro Reaction	7.14
7.3.5	Benzoin Condensation	7.15
7.3.6	Perkin Reaction	7.15
7.4	Qualitative tests for Aldehydes and Ketones	7.16
7.4.1	2, 4-DNP Test for Aldehydes and Ketones	7.17
7.4.2	Tollen's Test for Aldehydes	7.17
7.4.3	Jones (Chromic Acid) Oxidation Test for Aldehydes	7.18
7.4.4	Iodoform Test for Methyl Ketones	7.19
7.5	Structures and Uses of some Carbonyl Compounds	7.19
	• Questions	7.28



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Unit V

8. Carboxylic Acids (Aromatic and Aliphatic)

8

- 8.1 Introduction
- 8.2 Acidity of Carboxylic Acids
- 8.3 Effect of Substituents on Acidity
- 8.4 Inductive Effect
- 8.5 Qualitative Test for Carboxylic Acid ($R-/Ar-COOH$)
- 8.6 Structures and Uses of some Carboxylic Acids and Derivatives
 - Questions

9. Aliphatic Amines

9

- 9.1 Introduction
- 9.2 Basicity of Amines
- 9.3 Effects of Substituents on Basicity of Amines
- 9.4 Qualitative Tests for Amines
- 9.5 Structure and Uses of some Amines
 - Questions

Index

■ ■ ■



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Chapter ... 1

CLASSIFICATION, NOMENCLATURE AND ISOMERISM

♦ LEARNING OBJECTIVES ♦

- To know different types of Classes and Organic Compounds.
- To understand the IUPAC Rules for Nomenclature of Organic Compounds.
- To draw the Structure from given name.
- To give the name for given Structure.
- To understand types of Isomerism of the Organic Compound.

1.1 CLASSIFICATION OF ORGANIC COMPOUNDS

Classification of organic compounds on the basis of functional group and elemental composition:

1. Compounds containing carbon and hydrogen atoms only: Hydrocarbons (Alkanes, Alkenes, Alkynes, Aromatic Hydrocarbons, Arylalkyl Hydrocarbons, Alicyclic Hydrocarbons).
2. Compounds containing carbon, hydrogen and oxygen atoms only: Alcohols, Phenols, Ethers, Epoxides, Carbonyl compounds, Aldehydes and Ketones, Carboxylic acids, Esters, Anhydrides.
3. Compounds containing Carbon, Hydrogen and Nitrogen atoms only: Amines and Imines, Nitriles, Hydrazines.
4. Compounds containing Carbon, Hydrogen, Halogens with or without Oxygen: Alkyl Halides, Aryl Halides, Acyl Halides.
5. Compounds containing Carbon, Hydrogen, Oxygen and Nitrogen atoms only: Amides, Imides, Aldoximes, Ketoximes, Nitro compounds.
6. Compounds containing Carbon, Hydrogen and Sulphur with/without Nitrogen, Oxygen and Halogen: Sulphonic acids, Sulphonylhalides, Sulphonamides.
7. IUPAC nomenclature of all classes of compounds; Nomenclature of Mono-substituted and Poly-substituted compounds. (Recent rules of IUPAC referred).



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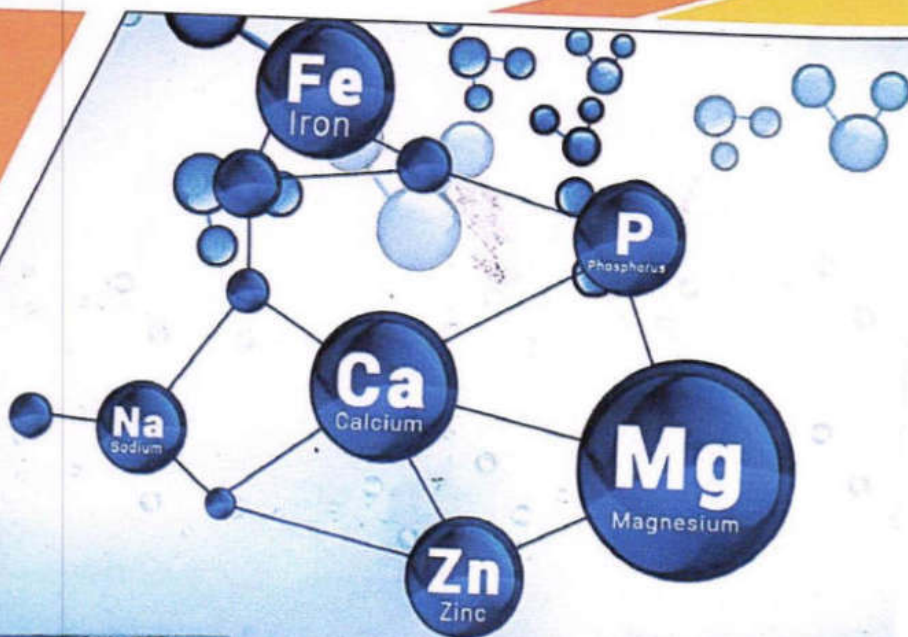
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Contents

1. Limit Tests for Various Ions - Introduction	1.1 - 1.26
1. To perform Limit Test for Chloride	1.2
2. To perform modified Limit Test for Chloride.	1.4
3. To perform Limit Test for Sulphate	1.5
4. To perform modified Limit Test for Sulphate	1.7
5. To perform Limit Test for Iron	1.8
6. To perform Limit Test for Lead	1.11
7. To perform Limit Test for Arsenic	1.15
8. To perform modified Limit Test for Arsenic	1.17
9. To perform Limit Test for Heavy metals	1.21
2. Qualitative Analysis of Inorganic Substances	2.1 - 2.41
10. Magnesium Hydroxide	2.22
11. Ferrous Sulphate	2.25
12. Sodium Bicarbonate	2.29
13. Calcium Gluconate	2.33
14. Copper Sulphate	2.36
3. Tests for Purity	3.1 - 3.6
15. To determine the neutralizing capacity of Aluminium Hydroxide Gel	3.1
16. To determine the Swelling Power of Bentonite	3.2
17. To determine Potassium Iodate and Iodine in Potassium Iodide	3.2
4. Preparation of Inorganic Pharmaceuticals	4.1 - 4.4
18. To prepare Boric Acid	4.1
19. To prepare Ferrous Sulphate	4.2
20. To prepare Potash Alum	4.3

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Chapter 1 ...

Limit Tests

Limit Tests are quantitative or semi-quantitative tests designed to identify or control small quantities of impurities. These tests should be specific and sensitive.

Limit = A value or amount that is likely to be present in a substance.

Test = To examine or to investigate

Impurity = A foreign matter present in a compound

Definition:

Limit test is defined as a quantitative or semi-quantitative test designed to identify and control small quantities of impurities which are likely to be present in the substance.

Importance of Limit Tests:

1. To find out the harmful amount of impurities
2. To find out avoidable / unavoidable amount of impurities.

Types of Limit Tests:

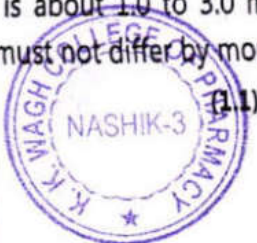
1. Comparison method
2. Quantitative determination
3. Test in which there is no visible reaction

General Principles:

1. If the sample is lighter (in colour/turbidity/opalescence) than the standard solution then it is within the pharmacopoeial limit (accepted).
2. If the sample is darker/heavier than the standard solution then it is above the pharmacopoeial limit (rejected).
3. **Specificity of a Limit Test:** A given limit test for a trace impurity should involve some selective reaction of the reagent with the trace impurity under consideration/detection specifically characteristic only to it.
4. **Sensitivity of a Limit Test:** As most of the limit tests involve dilute solutions and results are based on concentration of the trace impurity, the results may take longer duration to become observable or appreciable. Thus, consideration of duration of test needs to be of prime consideration in designing the limit test.

Nessler's Cylinder (IP appendix VII A127):

It is a clear glass cylinder with normal capacity of 50 ml. However, some Nessler's cylinders are of 100 ml capacity. The overall height is about 15 cm, the external height to the 50 ml mark is 11.0 to 12.4 cm and the thickness of the wall is around 1.0 to 1.5 mm, while, the thickness of the base is about 1.0 to 3.0 mm. The external height to the 50 mark of cylinders used for the test must not differ by more than 1 mm in the given pair.




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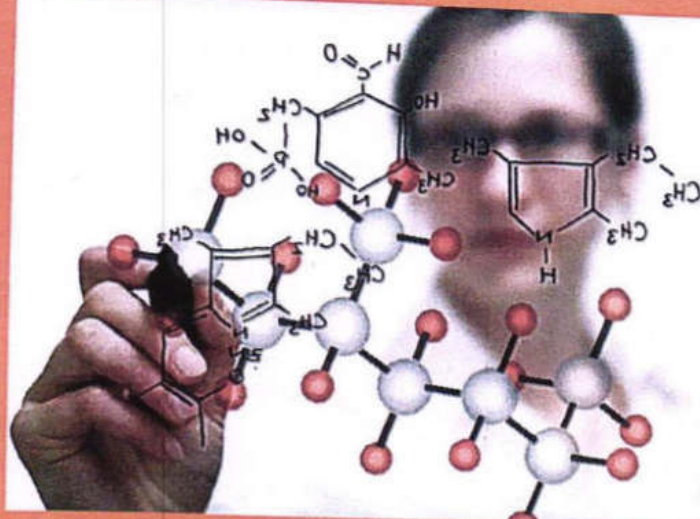
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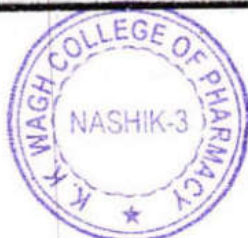
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Contents ...

1. Stereoisomerism	1.1 – 1.34
1.1 Introduction	1.1
1.2 Stereoisomerism	1.3
1.2.1 Configurational Isomerism	1.3
1.2.2 Conformational Isomerism	1.4
1.3 Optical Isomerism	1.4
1.4 Optical Activity	1.5
1.5 Molecular Symmetry and Chirality	1.7
1.6 Optical Isomers	1.9
1.6.1 Enantiomers and Diastereomers	1.9
1.7 DL System of Nomenclature of Optical Isomers	1.13
1.8 RS System of Nomenclature of Optical Isomers	1.15
1.9 Reactions of Chiral Molecules	1.23
1.9.1 The Stereochemistry of SN2 and SN1 Reactions	1.23
1.9.2 The Stereochemistry of E1 and E2 Reactions	1.24
1.10 Racemic Modification and Resolution of Racemic Mixture	1.27
1.11 Asymmetric Synthesis (Stereoselective Synthesis or the Synthesis of Chiral Molecules)	1.30
• Questions	1.32
2. Geometrical Isomerism	2.1 – 2.30
2.1 Introduction	2.1
2.2 Nomenclature of Geometrical Isomers	2.2
2.3 Methods of Determination of Configuration of Geometrical Isomers	2.6
2.3.1 Chemical Methods	2.6
2.3.2 Physical Methods	2.7
2.4 Conformational Isomerism	2.9
2.4.1 Newmann Projections	2.9
2.4.2 Sawhorse Projections	2.10
2.4.3 Conformational Isomerism and Conformational Analysis	2.10
2.4.4 Conformations of Ethane	2.11
2.4.5 Conformations of Butane	2.12
2.4.6 Conformations of Cyclohexane	2.14
2.4.7 Equatorial and Axial Bonds in Chair form of Cyclohexane	2.14
2.4.8 Conformation of Cyclohexane - Conformational Analysis	2.20
2.5 Stereo Isomerism in Biphenyl Compounds (Atropisomerism) and Conditions for Optical Activity	2.22
2.6 Stereoselective and Stereospecific Reactions	2.24
• Questions	2.28



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3. Heterocyclic Compounds - I

3.1 - 3.26

3.1	Introduction	3.1
3.2	Nomenclature of Heterocyclic Compounds	3.2
3.3	Classification of Heterocyclic Compounds	3.3
3.4	Pyrrole	3.8
3.4.1	Structure	3.8
3.4.2	Physical Properties	3.9
3.4.3	Synthesis of Pyrroles	3.9
3.4.4	Chemical Reactions	3.11
3.4.5	Medicinal uses of Pyrrole	3.14
3.5	Furan	3.15
3.5.1	Structure	3.15
3.5.2	Physical Properties	3.15
3.5.3	Synthesis of Furan	3.15
3.5.4	Chemical Reactions	3.16
3.5.5	Medicinal uses of Furan	3.19
3.6	Thiophene	3.20
3.6.1	Structure	3.20
3.6.2	Physical Properties	3.21
3.6.3	Synthesis of Thiophene	3.21
3.6.4	Chemical Reactions	3.21
3.6.5	Medicinal uses of Thiophene	3.22
3.7	Relative Aromaticity and Reactivity of Pyrrole, Furan and Thiophene	3.24
•	Questions	3.25

4. Heterocyclic Compounds - II

4.1 - 4.46

4.1	Pyrazole	4.1
4.1.1	Structure	4.1
4.1.2	Physical Properties	4.1
4.1.3	Synthesis of Pyrazole	4.1
4.1.4	Chemical Reactions	4.2
4.1.5	Medicinal uses of Pyrazole	4.3
4.2	Imidazole	4.4
4.2.1	Structure	4.4
4.2.2	Physical Properties	4.4
4.2.3	Synthesis of Imidazole	4.5
4.2.4	Chemical Reactions	4.6
4.2.5	Medicinal uses of Imidazole	4.11
4.3	Oxazole	4.12
4.3.1	Structure	4.12
4.3.2	Physical Properties	4.12
4.3.3	Synthesis of Oxazole	4.13
4.3.4	Medicinal uses of Oxazole	4.14



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K. K. Wagh College of Pharmacy
Nashik-422 003

4.4	Thiazole	4.15
4.4.1	Structure	4.15
4.4.2	Physical Properties	4.16
4.4.3	Synthesis of Thiazole	4.16
4.4.4	Chemical Reactions	4.16
4.4.5	Medicinal uses of Thiazoles	4.17
4.5	Pyridine	4.18
4.5.1	Structure and Physical Properties	4.18
4.5.2	Electrophilic Attack at Positions 3 and 5	4.18
4.5.3	Synthesis of Pyridine	4.19
4.5.4	Chemical Properties	4.20
4.5.5	Medicinal uses of Pyridine	4.23
4.6	Quinoline	4.24
4.6.1	Structure, Reactivity and Orientation	4.24
4.6.2	Synthesis of Quinoline	4.25
4.6.3	Chemical Properties	4.28
4.6.4	Medicinal uses of Quinoline	4.31
4.7	Isoquinoline	4.31
4.7.1	Structure	4.31
4.7.2	Physical Properties	4.31
4.7.3	Synthesis of Isoquinoline	4.32
4.7.4	Chemical Reactions	4.32
4.7.5	Medicinal uses of Isoquinoline	4.34
4.8	Acridine	4.35
4.8.1	Structure	4.35
4.8.2	Physical Properties	4.35
4.8.3	Synthesis of Acridine	4.35
4.8.4	Chemical Reactions	4.35
4.8.5	Medicinal uses of Acridine	4.36
4.9	Indole	4.36
4.9.1	Structure	4.36
4.9.2	Physical Properties	4.36
4.9.3	Synthesis of Indole	4.37
4.9.4	Chemical Reactions of Indole	4.39
4.9.5	Medicinal uses of Indole	4.41
4.10	Basicity of Pyridine	4.42
4.11	Pyrimidine	4.43
4.11.1	Synthesis of Pyrimidine	4.43
4.11.2	Pyrimidine: Biological Activity	4.44
4.12	Purine	4.44
	• Questions	4.45



5. Reactions of Synthetic Importance

- 5.1 Metal Hydride reduction by Sodium Borohydride (NaBH_4) and Lithium Aluminium Hydride (LiAlH_4)
- 5.2 Clemmensen Reduction
- 5.3 Wolf Kishner Reduction
- 5.4 Birch Reduction
- 5.5 Oppenauer-Oxidation
- 5.6 Dakin Reaction
- 5.7 Claisen-Schmidt Condensation
- 5.8 Schmidt Rearrangement
- 5.9 Beckmann Rearrangement
- Questions

5.1
5.4
5.6
5.7
5.8
5.10
5.11
5.13
5.14
5.15



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Unit ... 1

STEREOISOMERISM

♦ LEARNING OBJECTIVES ♦

After completing this chapter, reader should be able to understand:

- Optical isomerism – Optical Activity
- Enantiomerism
- Diastereoisomerism
- Meso Compounds
- Elements of Symmetry
- Chiral and Achiral Molecules
- DL System of Nomenclature of Optical Isomers, Sequence Rules
- RS System of Nomenclature of Optical Isomers
- Reactions of Chiral Molecules
- Racemic Modification and Resolution of Racemic Mixture
- Asymmetric Synthesis: Partial and Absolute

1.1 INTRODUCTION

Stereochemistry is a branch of organic chemistry which deals with structure of compounds in three dimensions and hence can be termed as chemistry or study of compounds with respect to the arrangements and movements of different atoms or group of atoms in space. The word is derived from Greek word (Stereos = "three"-dimensionality).

Stereochemistry also deals with stereo-isomerism and stereo-chemical reactions of organic compounds.

Founders of Stereochemistry:

		
Biot realized in 1815 that the solutions of many naturally occurring compounds rotate the plane of polarization of plane polarized light.	Pasteur recognized in 1850 that the optical activity was caused by an asymmetric arrangement of atoms in a molecule.	van't Hoff with Le Bel described in 1874 how the atoms of a molecule are actually arranged in space.

Fig. 1.1: Founders of Stereochemistry

(1.1)



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Contents ...

1. Introduction to Pharmaceutical Substances	1.1 - 1.32
2. Acids Bases and Buffers	2.1 - 2.12
3. Major Extra and Intracellular Electrolytes	3.1 - 3.20
4. Dental Products	4.1 - 4.10
5. Gastrointestinal Agents	5.1 - 5.4
6. Antacids	6.1 - 6.14
7. Cathartics	7.1 - 7.6
8. Antimicrobials	8.1 - 8.10
9. Miscellaneous Agents	9.1 - 9.14
10. Radiopharmaceuticals	10.1 - 10.14



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Chapter 1 ...

Impurities in Pharmaceutical Substances

Contents ...

- 1.1 Inorganic Chemistry
 - 1.1.1 Importance of Inorganic Pharmaceuticals
- 1.2 Pharmacopoeia
 - 1.2.1 History of Pharmacopoeia
 - 1.2.2 Indian Pharmacopoeia
 - 1.2.3 Indian Pharmacopoeia 2010
 - 1.2.4 Indian Pharmacopoeia 2014
 - 1.2.5 Indian Pharmacopoeia 2018
 - 1.2.6 British Pharmacopoeia
 - 1.2.7 European Pharmacopoeia
 - 1.2.8 Pharmacopoeia International (International Pharmacopoeia)
 - 1.2.9 United States Pharmacopoeia (USP)
- 1.3 Official Monograph
- 1.4 New Inclusion / Exclusion of Monograph
- 1.5 Sources of Impurities
- 1.6 Limit Tests
 - 1.6.1 Limit Test for Chlorides
 - 1.6.2 Limit Test for Sulphates
 - 1.6.3 Limit Test for Iron
 - 1.6.4 Limit Test for Lead
 - 1.6.5 Limit Test for Heavy Metals
 - 1.6.6 Limit Test for Arsenic
 - 1.6.7 Limits of Insoluble and Soluble Matter
- 1.7 Qualitative Tests for Alkali and Alkaline Earth Metals
- 1.8 Modified Limit Tests for Chlorides and Sulfates
- Question Bank



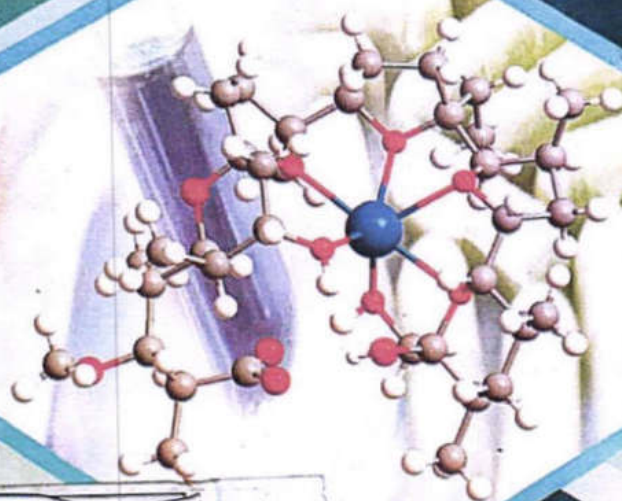
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Contents

Unit I

1. Benzene and Its Derivatives

1.1 – 1.22

- | | | |
|-----|--|------|
| 1.1 | Structure of Benzene | 1.1 |
| 1.2 | Analytical Evidences | 1.2 |
| 1.3 | Synthetic/Chemical Evidences | 1.2 |
| 1.4 | Orbital Picture of Benzene | 1.3 |
| 1.5 | Resonance and Aromaticity in Benzene | 1.4 |
| 1.6 | Reactions of Benzene | 1.6 |
| 1.7 | Electrophilic Aromatic Substitution | 1.7 |
| 1.8 | Nucleophilic Aromatic Substitution | 1.17 |
| 1.9 | Structure and Uses of some selected Benzene Derivatives,
viz., DDT, Saccharin, BHC and Chloramine | 1.18 |
| • | Questions | 1.22 |

Unit II

2. Phenols

2.1 – 2.13

- | | | |
|-----|------------------------|------|
| 2.1 | Introduction | 2.1 |
| 2.2 | Acidity of Phenols | 2.2 |
| 2.3 | Methods of Preparation | 2.3 |
| 2.4 | Reactions of Phenols | 2.6 |
| • | Questions | 2.13 |

3. Aromatic Amines

3.1 – 3.14

- | | | |
|-------|--|-----|
| 3.1 | Introduction | 3.1 |
| 3.2 | Methods of Preparation | 3.2 |
| 3.3.1 | Reduction of Nitriles | 3.2 |
| 3.2.2 | Reduction of Nitrocompounds | 3.2 |
| 3.2.3 | Selective Reduction by Ammonium Sulphide | 3.3 |
| 3.2.4 | Reductive Amination of Ketone | 3.3 |
| 3.2.5 | Hoffmann Rearrangement | 3.3 |
| 3.2.6 | Ammonolysis of Aryl Chloride | 3.3 |
| 3.3 | Chemical Reactions of Aromatic Amines | 3.3 |
| 3.3.1 | Formation of Amide from Acyl Chloride | 3.3 |
| 3.3.2 | Salt Formation | 3.4 |
| 3.3.3 | Reaction with Nitrous Acid | 3.4 |
| 3.3.4 | Carbylamine Reaction | 3.4 |
| 3.3.5 | Acetylation | 3.5 |
| 3.3.6 | Reaction with Aldehydes (Schiff's Base) | 3.5 |
| 3.3.7 | Oxidation Reactions | 3.5 |



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Nashik-422 003

3.4	Basicity of Amines	3.5
3.5	Effects of Substituents on Basicity of Amines	3.7
3.6	Factors affecting on Basicity	3.7
3.6.1	Resonance Effect	3.8
3.6.2	Inductive Effect	3.8
3.6.3	Hydrogen Bonding	3.9
3.6.4	Orbital Nature of Electron Pair	3.9
3.6.5	Steric Effect	3.9
3.6.6	Solvation Effect	3.9
3.6.7	Electronegativity of Bonded Atoms	3.10
3.7	Aryl Diazonium Salts	3.10
3.7.1	History of Aryl Diazonium Salts	3.10
3.7.2	Aryl Diazonium Salts	3.10
3.7.3	Preparation of Benzenediazonium Chloride	3.11
3.7.4	Synthetic Applications of Aryl Diazonium Salts	3.12
3.7.5	Importance of Diazonium Salts	3.13
•	Questions	3.14
4.	Aromatic Acids	4.1 – 4.8
4.1	Introduction	4.1
4.2	Acidity: Salt Formation	4.2
4.3	Important Reactions of Benzoic Acid	4.3
4.4	Methods of Preparation of Aryl Carboxylic Acids	4.6
•	Questions	4.8

Unit III

5.	Fats and Oils	5.1 – 5.6
5.1	Introduction	5.1
5.2	Reactions of Fatty Acids	5.2
5.2.1	Hydrolysis	5.2
5.2.2	Hydrogenation	5.2
5.3	Rancidity of Oil (Rancidification)	5.2
5.3.4	Drying Oils	5.3
5.3	Principles and Significance of various Analytical Constants	5.3
5.3.1	Acid Value	5.4
5.3.2	Saponification Value	5.4
5.3.3	Ester Value	5.5
5.3.4	Iodine Value	5.5
5.3.5	Acetyl Value	5.6
5.3.6	Reichert-Meissl (RM) Value	5.6
•	Questions	5.6



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Unit IV**6. Polynuclear Hydrocarbons****6.1 – 6.24**

6.1	Introduction	6.1
6.2	Naphthalene	6.1
6.2.1	Synthesis of Naphthalene	6.3
6.2.2	Properties	6.4
6.2.3	Chemical Reactions	6.6
6.2.4	Uses of Naphthalene and its Derivatives	6.9
6.2.5	Structures of Naphthalene Derivatives	6.10
6.3	Anthracene	6.10
6.3.1	Synthesis	6.11
6.3.2	Chemical Reactions	6.12
6.3.3	Uses of Anthracene and its Derivatives	6.14
6.3.4	Structures of Anthracene Derivatives	6.15
6.4	Phenanthrene	6.16
6.4.1	Synthesis	6.16
6.4.2	Chemical Reactions	6.19
6.4.3	Uses of Phenanthrene and its Derivatives	6.20
6.5	Diphenylmethane (Benzylbenzene)	6.21
6.6	Triphenylmethane	6.21
•	Questions	6.24

Unit V**7. Cycloalkanes****7.1 – 7.7**

7.1	Introduction	7.1
7.2	Classification of Saturated Cycloalkanes	7.1
7.3	Methods of Preparation of Cycloalkanes	7.3
7.3.1	From Dihalides	7.3
7.3.2	Dieckmann Reaction	7.3
7.3.3	Simmons-Smith Reaction	7.3
7.3.4	From Aromatic Hydrocarbon	7.3
7.4	Stability of Cycloalkanes	7.4
7.4.1	Baeyer Strain Theory	7.4
7.4.2	Sache-Mohr's Theory of Strainless Rings	7.5
7.5	Reactions of Cyclopropane and Cyclobutane	7.6
7.5.1	Substitution Reactions	7.6
7.5.2	Addition of Cl_2 and Br_2	7.6
7.5.3	Addition of HBr and HI	7.6
7.5.4	Addition of Hydrogen	7.6
•	Questions	7.7


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Unit I

Chapter ... 1

BENZENE AND ITS DERIVATIVES

♦ LEARNING OBJECTIVES ♦

After completing this chapter, reader should be able to understand:

- Introduction to benzene.
- Analytical, Synthetic and other evidences in the derivation of structure of benzene.
- Orbital picture of benzene.
- Resonance in benzene, aromatic characters, Huckel's rules.
- Reactions of benzene - nitration, sulphonation, halogenation-reactivity, Friedel-Crafts alkylation - reactivity, limitations, Friedel-Crafts acylation.
- Substituents, effect of substituents on reactivity and orientation of mono substituted benzene compounds towards electrophilic substitution reaction.
- Structure and uses of DDT, Saccharin, BHC and Chloramine.

1.1 STRUCTURE OF BENZENE

Benzene on which the study of aromatics began was discovered in 1825. However, it was not till 1866 that the Kekule's formula or structure I of benzene was known, till he proposed it. This structure of benzene is most accepted because the satisfactory answers it offers to various substitution products as compared with other four proposed structures II-V (Fig. 1.1.).

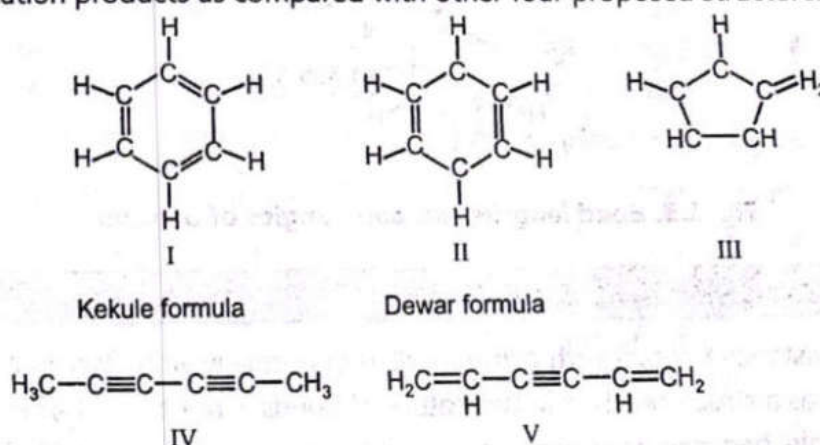
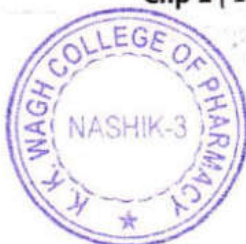


Fig. 1.1: Various structures proposed for benzene in earlier days

Chp 1 | 1.1



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3.3.2

B. Papers published in national/ international conference proceedings



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3.3. Research Publications and Awards

3.3.2 Number of books and chapters in edited volumes/books published and papers published in national/ international conference proceedings per teacher during last five year

B. Papers published in national/ international conference proceedings

Sr. No.	Name of the teacher	Title of the paper	Title of the proceedings of the conference	National / International	Year of publication	Affiliating Institute at the time of publication
1	Dr. Amrutkar R. D, Kadam D. K, Dr. Jain K. S.	Design, Synthesis and evaluation of novel RTK-inhibitors as potential anticancer agents.	RAKCOPS International Conference on Drug Development 2021	International	2021	K. K. Wagh College of Pharmacy



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RAK Medical & Health Sciences University
Ras Al Khaimah, United Arab Emirates



RAK College of Pharmaceutical Sciences

RAKCOPS International e-Conference on Drug Development 2021

Certificate of Appreciation

This Is To Certify That

Dr. RAKESH DEVIDAS AMRUTKAR

Has Presented Professional e-Flash Talk At RAKCOPS-ICDD 2021 e-Conference, May 23-24, 2021

Title: Design, synthesis and evaluation of novel RTK-inhibitors as potential anticancer agents

Authors: Amrutkar R. D., Kadam D. K., Jain K. S.

Dr. Bhoomendra Bhongade
Chief Coordinator

Dr. Padma GM Rao
Dean, RAKCOPS

Dr. S. Gurumadhva Rao
President, RAKMHSU

**RAKCOPS-ICDD
2021**



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RAKCOPS/ICDD-PC122-F21



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2021

Abstract Book

RAKCOPS International e-Conference on Drug Development 2021

RAKCOPS-ICDD 2021

Theme:

Quality Medicines from Bench to Bed Side

May 23-24, 2021

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e-FLASH TALKS

PC104-F	Immunoinformatics approach for a novel multi-epitope vaccine construct against spike protein of human coronaviruses Avinash Kumar, Ekta Rath, Suvama G. Kini	29
PC106-F	Synthesis and pharmacological evaluation of some substituted imidazoles on indole moiety Kshirsagar S.S., Chavan R.S., Amnerkar N.D., Bhusari K.P.	30
PC107-F	Meta-dynamics based ensemble docking and virtual screening on SARS-Cov-2 RNA-dependent RNA-polymerase (RdRp) Prajata M. Phage*, Komal S. Pol, Rajesh B. Patil	31
PC122-F	Design, synthesis and evaluation of novel RTK-inhibitors as potential anticancer agents Amrutkar R. D.*, Kadam D. K., Jain K. S.	32
PC127-F	Development and validation of a stability indicating RP-HPLC method for the estimation of antidiabetics in combined pharmaceutical dosage form. Leena A. Sawalkar*, P. Kapupara	33
PC134-F	Simultaneous estimation of pioglitazone and its metabolites in human plasma by liquid chromatographic tandem mass spectrometric method Vig N.*, Jain G.K., Chopra S.	34
PT207-F	Comparative analysis of the efficacy of gemifloxacin mesylate and corticosteroids from ophthalmic ocuserts Keny S.M.*, Shah K.	35
PT218-F	Design and Characterization of Oral Drug Delivery System Using Pastillation Technique Suresh G. Sudke*, Nagesh H. Aloorkar, Pramod V. Burakale	36
PT231-F	Analysis of Daclatasvir Dissolution Kinetics using Ratio Tests Saima Quadri*, Syed Muhammad Farid Hasan, Monica Gautam Parkash Ojha	37
CPP306-F	Assessment of prescribing pattern in the coronary artery diseases in a tertiary care hospital - a retrospective study K. V. Ramanath*, Niloufar Emami, Alireza Lashani, Navya Shree	38
CPP311-F	To explore the effect of diosmin in acute myocardial infarction in experimental model Ritu Kainth*, Mohd Amin Ganie, Navpreet Singh, Ajay Singh Kushwah	39
CPP323-F	Investigation of mitigating effect of an osteoarthritic drug in inflammatory bowel disease through drug repurposing strategy Supriya Roy*, Suneela Dhaneshwar, Tarique Mahmood	40
CPP327-F	Active surveillance of hemovigilance in a tertiary care teaching hospital: a developing country scenario Amruta Ashok Poldar*, Pallavi P., M. Ramesh, Sri Harsha Chalasani	41
CPP328-F	Adherence to medication: Patient reported facilitators and barriers M. Ramesh, Abaka Mohith Kumar*, Fasil Majeed P. V., Patric Rejimon, Emelda Chinemerem	42





Poster Code: PC122-F

Title	: Design, synthesis and evaluation of novel RTK-inhibitors as potential anticancer agents
Author(s)	: <u>Amrutkar R. D., Kadam D. K., Jain K. S.</u>
Affiliation	: Department of Pharmaceutical Chemistry, K. K. Wagh College of Pharmacy, Nashik, Maharashtra, India. Email: rdamrutkar@kkwagh.edu.in
Introduction	: N.D.D.R. in the field cancer chemotherapy has RTKs (Receptor Tyrosine Kinases) as one of the most popular targets.
Objectives	: Design, green one-pot synthesis and evaluation of novel bioisosteres of gefitinib for antiproliferative activity on a various cell lines and lead optimization by various CADD techniques.
Materials & Method	: Novel condensed 2- <i>H</i> -pyrimidin-4-amines, as bioisosteric analogs of well-known antiproliferative anticancer drug gefitinib were designed and synthesized by one-pot MWI based synthesis. These compounds have been evaluated for antiproliferative & antitumour activities by <i>in-vitro</i> testing against 5 cancer cell lines [EAC (Ehrlich Ascites Carcinoma), A549 (Lung Carcinoma), HT-29 (Adenocarcinoma), MDA-MB 231 (Breast cancer) and HeLa (Cervix cancer) cell lines]. 3D-QSAR for the optimization of 3D structural features, done by COMFA, COMISIA and PHASE. Docking studies with GLIDE revealed good binding with RTK's.
Results and discussion	: Many compounds revealed excellent potential as anticancer NCEs as the PIC ₅₀ values of some are better than that for gefitinib. 3D-QSAR study for the optimization of 3D structural features, done by COMFA, COMISIA and PHASE. Docking studies with GLIDE revealed good binding with RTK's.
Conclusion	: As the PIC ₅₀ values of some compounds are better than that obtained for gefitinib so the compounds have revealed excellent potential to be developed as anticancer drugs. Further, docking studies also reveals good binding with RTK's.

