SARVAJANIK UNIVERSITY
M.Sc. Organic Chemistry Syllabus (CBCS)
FOURTH SEMESTER

Program: M.Sc.	**Type:** Theory
Subject: DSC- VII: Physical Organic Chemistry	
Credit: 04(T) + 02 (P)	**Total learning hours:** 60
Course description: This course paper covers thermodynamic and kinetic requirements of organic reaction – reactivity, reaction mechanism, study of acidity and basicity of organic compounds, mechanisms of surface reactions, application of chemical kinetics in pharmaceuticals, molecular dynamics in biological macromolecules.	
Student learning outcome: At the end students will be able to learn about…. • Thermodynamic and Kinetic requirements of organic reaction • Reactivity and selectivity principles • Determination of Reaction Mechanism • Linear free energy relationships (LFER) • Factors affecting acidity and basicity, Acid and base catalysis • Kinetic effects of surface heterogeneity & interactions • **C**alculation of elimination rate constant & metabolism constant • Supramolecular reactivity and catalysis • Molecular channels, devices and transport processes	

Unit 1 Thermodynamic and Kinetic Necessities of a Reaction **(06 Hours)**

1.1 Chemical equilibrium: rate and equilibrium constants
1.2 Mechanistic significance of entropy, enthalpy and Gibb's free energy
1.3 Arrhenius equation, transition state theory, uses of activation parameters
1.4 Transition state model- potential energy surface for substitution and elimination reactions

Unit 2 Principle of Reactivity **(06 Hours)**

2.1 Hammond's postulate, Marcus theory of electron transfer
2.2 Reactivity and selectivity principles,
2.3 Curtin-Hammett Principle, Microscopic reversibility
2.4 Kinetic *vs* thermodynamic control of organic reactions

Unit 3 Determination of Reaction Mechanism **(08 Hours)**

3.1 Product analysis, Kinetic studies
3.2 Theory of isotope effect: primary and secondary kinetic isotope effects
3.3 Heavy atom isotope effects, Tunnelling effect, Solvent effect
3.4 Detection and trapping of intermediates
3.5 Crossover experiments and stereochemical evidence

Unit 4 Structural Effects on Reactivity **(10 Hours)**

4.1 Linear free energy relationships (LFER)
4.2 The Hammett equation, substituent, constants
4.3 Theories of substituent effects, interpretation of σ values, reaction constant ρ

4.4 Deviations from Hammett equation, dual-parameter corrections, inductive substituent constant
4.5 The Taft model σ I - and σ R – scales, Swain-Scott & Edward equations, Winstein Grunwald relationship
4.6 Isokinetic relationship

Unit 5 Acids and Bases (06 Hours)

5.1 Factors affecting acidity and basicity: Electronegativity and inductive effect, resonance, bond strength, electrostatic effects, hybridization, aromaticity and solvation.
5.2 Comparative study of acidity and basicity of organic compounds on the basis of pKa values
5.3 Levelling effect and non-aqueous solvents
5.4 Acid and base catalysis - general and specific catalysis with examples

Unit 6 Reactions at Surfaces (06 Hours)

6.1 Mechanisms of surface reactions- kinetic effects of surface heterogeneity & interactions
6.2 Surface inhibition and activation energies - Surface exchange reactions– TST of surface reactions
6.3 Unimolecular & bimolecular reactions
6.4 Micelles: Surface active agents-micellization, CMC, micellar catalysis

Unit 7 Application of Chemical Kinetics in Pharmaceuticals (06 Hours)

7.1 Pharma concentration time curve
7.2 Protein binding and drugs, drug dissolution rate
7.3 Pharmacokinetics applied to one-component open model
7.4 **C**alculation of elimination rate constant & metabolism constant

Unit 8 Molecular Dynamics (12 Hours)

8.1 Principle of molecular association and organization in biological macromolecules:
8.1.1 Enzymes, nucleic acids, membranes
8.1.2 Model systems like micelles and vesicles
8.2 Molecular receptors and design principle
8.2.1 Cryptands, cyclophanes, calixeranes, cyclodextrines
8.3 Supramolecular reactivity and catalysis
8.4 Molecular channels and transport processes
8.5 Molecular devices and nanotechnology

References:

1. Molecular Mechanics, U. Burkert and N.L. Allinger, ACS Monograph 177, 1982
2. Physical Organic Chemistry, N.S. Isaacs, ELBS/Longman,1990.
3. Supramolecular Chemistry; Concepts and Perspectives, J.M. Lehn, 1995, VCH, Weinheim.
4. Physical Chemistry, Peter Atkins and Julio de Paula, 5th Edition, 2006, W. H. Freeman and Company New York.
5. Chemical Kinetics, Keith J. Laidler, 3rd Edition, 1987, Pearson Education.
6. The Physical Basis of Organic Chemistry, H. Maskill, 1985, Oxford University Press.
7. Catalysis, J.C. Kuriacose, 1991, Macmillan India Ltd.
8. Micelles, Theoretical and applied aspects, V. Moroi, 1992, Plenum.
9. Mechanism and Theory in Organic Chemistry, T.H. Lorry and K.S. Richardson, 2nd Edition, 1981, Harper & Row, New York.
10. A Guidebook to Mechanism in Organic Chemistry, P. Sykes, 5th Edition, 1981, Longman, London,.
11. L.P. Hammett, Physical Organic Chemistry, 2nd Edition, 1970, McGraw Hill, NewYork.
12. P. Deslongchamps, Stereoelectronic Effects in Organic Chemistry, 1983, Pergamon, London.

SARVAJANIK UNIVERSITY
M.Sc. Organic Chemistry Syllabus (CBCS)
FOURTH SEMESTER

Program: M.Sc.	**Type:** Theory
Subject: DSC-VIII: Industrial Chemistry	
Credit: 04(T)	**Total learning hours:** 60
Course description: This course paper includes the concept of material and energy balance, design of equipment, various instruments useful in industry, flow chemistry, industrial polymers, developments of process in chemical industries, strategies for organic reaction and processes and phase transfer catalysis.	
Student learning outcome: At the end the students will be able to learn about.. • Material and energy balance and calculations • Material and design of chemical reactor, pressure vessel • Instruments for measuring temperature, pressure and water flow of process stream • Principles and types of flow chemistry • Principle, working and applications of polymer processing techniques • Objectives and approaches of process development in chemical industries • Choice of reagents and solvents for organic reaction and processes • Nature and factors of phase transfer catalysis reactions	

Unit 1 Material and Energy Balance **(06 Hours)**

1.1 Material balance: Process classification
1.2 Choice of system and basis of molecular processes with chemical reactions
1.3 Material balance calculations
1.4 Multiple unit processes, Recycle and bypass
1.5 Energy balance: Forms of energy, Energy balance
1.6 Energy changes in physical processes
1.7 Energy changes in reactions
1.8 Energy balance Calculations

Unit 2 Equipment Design **(06 Hours)**

2.1 Material of constructions: Mechanical properties, Corrosion resistance
2.2 Plastics, Ceramics, Metals and alloys, Stainless steel
2.3 Special material for food and pharmaceutical equipment
2.4 Protective coatings, Surface treatment to metals for corrosion resistance
2.5 Classification of chemical reactors, Design of chemical reactors
2.6 Pressure vessels for internal or external pressure

Unit 3 Industrial Instrumentation **(06 Hours)**

3.1 Measurement of temperature, Thermo couples and pyrometers, High temperature thermometers
3.2 Optical pyrometers, Measurement of pressure and vacuum, Manometric and Bourdon gauges, Vacuum gauges, Ionization and pirani gauges
3.3 Flow measurement, Pitot tube, Rotameters, Liquid level indicators, Hook Type, Sight glass, Float type, Capacitance level indicator, Radiation level indicator

Unit 4 Flow Chemistry **(06 Hours)**

4.1 Introduction
4.2 Flow chemistry versus batch chemistry
4.3 Key principles of flow chemistry: residence time, mixing, pressure and temperature
4.4 Types of flow chemistry

Unit 5 Industrial Polymers **(08 Hours)**

5.1 Introduction
5.2 Principle, Working and applications of following polymer processing techniques: Injection moulding, extrusion, blow moulding, compression moulding, film casting, thermoforming and vacuum forming

Unit 6 Process Development in Chemical Industries **(12 Hours)**

6.1 Introduction to process research & development
6.2 Goals & Objectives of Process development
6.3 Stages in process development
6.4 Scope and Limitations of Process development
6.5 Exploratory (Investigative) approach in Process development
6.6 Survey of Some organic reactions in relation to process development

Unit 7 Strategies for simplification of organic reaction and processes **(06 Hours)**

7.1 Choosing a reagent, Modifying reagents
7.2 Solvents: choosing a solvent, impurities in solvent, effect of solvents in organic reactions, mixed solvents,
7.3 Aqueous mediums for organic reactions, liquid products as solvents, new solvents

Unit 8 Phase transfer catalysis **(10 Hours)**

8.1 Nature of phase transfer catalysis reactions
8.2 Factors effecting phase transfer catalysis reactions
8.3 Choosing a phase transfer catalyst
8.4 Important phase transfer catalysts

References:

1. Industrial chemistry, H.K. L. Vaid, 1st Edition, 2007, Anmol publication.
2. Fundamentals of Industrial Chemistry: Pharmaceuticals, Polymers, and Business, John A. Tyrell, 2014.
3. Outlines of industrial chemistry, Frank Hall Thorp and Warren Kendall Lewis, 2018, Palala Press.
4. Industrial Chemistry, Dr. Darshan V. Chaudhary, 1st Edition, 2015, Create space publisher.
5. Industrial Inorganic Chemistry, Mark Anthony Benvenuto, de Gruyter, 2013.
6. Organic Chemistry Principles and Industrial Practice, Mark M. Green , Harold A. Wittcoff, 1st Edition, Willey-VCH Gmbh & Co, KGaA.
7. Toma Glasnov, Continuous-Flow Chemistry in Research Laboratory, Springer International Publisher.

8. Polymer Technology, D.C. Miles & J. H. Briston, Enlarged edition, 1996, Chemical Publishing company, Inc, New York
9. Plastics Materials and Processes, Seymour S. Schwartz S.H. Goodman,1982, Van Nostrand Reinhold, New York
10. Plastics Technology, R. V. Milbey, 1st Edition, 1973, McGraw Hill, Book Company New York
11. The chemistry of process development in fine chemicals and pharmaceutical industry, C. Someshwara Rao, 2nd Edition, 2004, Asian books Pvt. Ltd. New Delhi
12. Developing an Industrial chemical process, Joseph Mizrahi, 2003, CRC press
13. Practical process research and development, N. G. Anderson, 2000, American Press
14. Designing and operating safe chemical reaction process, Health and Safety Executive (HSE), 2000, HSE publishers

SARVAJANIK UNIVERSITY
M.Sc. Organic Chemistry Syllabus (CBCS)
FOURTH SEMESTER

Program: M.Sc. Organic Chemistry	**Department:** Chemistry
Semester: IV	**Type:** Theory
Subject: DSE-V-Principles of Medicinal Chemistry	
Credit: 04(T)	**Total learning hours:** 60
Course description: This course explores the role of organic chemistry in the discovery and synthesis of important compounds widely used as medicines. It includes drug discovery process, QSAR concept, and role of computer in drug design. This syllabus also covers pharmacokinetics and pharmacodynamics which is very important for the students of medicinal chemistry. Apart from these some important drugs are also discussed in this paper.	
Student learning outcome: At the end of the course…… • Students will gain a comprehensive understanding of the fundamental concepts related to the actions and clinical uses of major classes of drugs from their chemical structures • They will be familiar with history of drugs, new invention in Medicinal chemistry • Students will get an overview of the applications of these concepts in applied field • Students will be aware about the basic ideas of medicines & their working mechanism • Students will have knowledge of synthesis of some drugs	

Unit-1 Introduction to Drug Discovery **(10 Hrs)**

1.1 Introduction
1.2 Stereochemistry and drug design
1.2.1 Structurally rigid groups
1.2.2 Conformation
1.2.3 Configuration
1.3 Solubility and drug design
1.4 Solubility and drug structure
1.5 Salt formation
1.6 The incorporation of water solubilizing groups in a structure
1.6.1 The type of group
1.6.2 Reversibly and irreversibly attached groups
1.6.3 The position of the water solubilizing group
1.6.4 Methods of introduction

Unit-2 Quantitative Structure–Activity Relationship **(08 Hrs)**

2.1 Introduction to quantitative structure activity relationship studies
2.2 Lipophilicity
2.2.1 Partition coefficients (P)
2.2.2 Lipophilic substitution constants
2.3 Electronic effects: The Hammett constant (s)
2.4 Steric effects
2.4.1 Taft steric parameter (Es)
2.4.2 Molar refractivity (MR)
2.4.3 Other parameters
2.5 Hansch analysis
2.6 Craig plots
2.7 Topliss decision tree

Unit-3 Computer Aided Drug Design **(07 Hrs)**

3.1 Introduction
3.1.1 Molecular modelling methods
3.1.2 Computer graphics
3.2 Molecular mechanics
3.2.1 Creating a molecular model using molecular mechanics
3.3 Molecular dynamics
3.3.1 Conformational analysis
3.4 Quantum mechanics
3.5 Docking

Unit-4 Pharmacokinetic **(07 Hrs)**

4.1 Basic principles of pharmacokinetics
4.1.1 Absorption
4.1.2 Distribution
4.1.3 Metabolism
4.1.4 Excretion
4.2 Pharmacokinetic models
4.3 Pharmacokinetic parameters in defining drug deposition and in therapeutics
4.4 Uses of pharmacokinetics in drug development process
4.5 Concept of pro drug and soft drug

Unit-5 Pharmacodynamics **(08 Hrs)**

5.1 Introduction
5.2 Principles of drug action
5.3 Mechanisms of drug action
5.4 Introduction to the concept of receptors and drug receptor interactions
5.5 Biotransformation
5.6 Dose-response relationships
5.7 Drug potency and efficacy
5.8 Combined effect of drugs

Unit-6 Antibiotics **(07 Hrs)**

6.1 Introduction and classification
6.2 Antibiotics that interfere with the biosynthesis of bacterial cell wall
6.2.1 The β -lactum antibiotics: Penicillin and Cephalosporin (Synthesis and uses)
6.2.2 Non lactum antibiotics
6.2.3 Bacitracin, Vancomycin and Cycloserine (Synthesis and therapeutic uses)
6.3 Antibiotics that interfere with the protein biosynthesis in microorganisms
6.3.1 Non lactum antibiotics: Tetracycline, Chloroamphenicol
6.4 Non classifiable antibiotics

Unit-7 Drugs Acting at Synaptic and Neuro-Effector Junction Sites **(07 Hrs)**

7.1 Cholinergics and Anticholinesterases
7.2 Adrenergic .drugs

7.3 Antispasmodic and antiulcer drugs
7.4 Neuromuscular blocking agents

Unit-8 Miscellaneous **(06 Hrs)**

8.1 Antifungal – polyenes
8.2 Antiviral – Acyclovic
8.3 Antimalarials : : Modern chemotherapy of malaria, 4-amino and 8-amino quinolins, 9- amino acridine
8.4 Mode of action of antimalarial agents
8.5 SAR of antimalarial agents
8.6 Synthesis of mefloquines, chloroquine, primaquine and daraprim

Reference:

1. Burger's medicinal chemistry and drug design, 1997, vol 1 to 5 edited by Manfred E.Woltt John wiley and sons Mc. New York
2. Foye's Principles of medicinal chemistry, Thomas Lemke, 2012, Lippincott Williams and Wilkins
3. Principles of medicinal chemistry vol I & II (5/e), F.S.kadam, K.R. Mahadic ad K.G.Bohra, 2019, Nirali publication
4. Medicinal chemistry, Ashutosh kar, 2018, New Age International Publishers
5. The organic chemistry of drug synthesis vol I, II and III Daniel Lednicer (Editor), Lester A. Mitscher (Editor), 1980, Wiley
6. An introduction to Medicinal chemistry, G. L. Patrick, 2018, Oxford University Press
7. The Organic Chemistry of Drug Design and Drug Action, Richard B. Silvermann, 2014, Academic Press
8. Essentials of Medical Pharmacology, K. D. Tripathi, 2019, Jaypee Brothers Medical Publishers (P) Ltd.
9. A textbook of medicinal chemistry, P. Primoo, 2019, CBS Publishers & Distributors
10. Text book of pharmaceutical organic chemistry, Md. Ali, 2020, CBS Publishers

SARVAJANIK UNIVERSITY
M.Sc. Organic Chemistry Syllabus (CBCS)
FOURTH SEMESTER

Program: M.Sc.	**Type:** Theory
Semester-4	
Subject: DSE – IV Dyes	
Credit: 04(T)	**Total learning hours:** 60

Course description:
This course will give an introduction to dyes and pigments. The primary goal of this course is to make students aware of how dyes can be classified and the basic chemistry applied in dyeing process. This subject provides fundamental knowledge of various types of dyes and how to carry out dyeing process in textile industries. This course also includes applications of dyes in the field other than textile fibres.

Student learning outcome:
Upon completion of this course, students will be able to learn about:

- To explain the and define the classes of dyes, substrates
- To understand the variety and chemistry of dyes and their application
- To distinguish the various dye class and their application to different fibres types
- To understand the uses of dyes in non-textile field.

Unit 1 Colour and constitutions **(06 Hours)**

1.1 Colour, chromophore and Auxochromes.
1.2 Classification of dyes based on chemical nature.
1.3 Relation between colour and constitution
- 1.3.1 Witt's theory
- 1.3.2 Armstrong theory
- 1.3.3 Modern theory
  - (a)Valence bond theory
  - (b)Molecular orbital theory

Unit2 Dyes **(08 Hours)**

2.1 Definition, Classification Based on Application
2.2 Fastness properties & applicability on substrates
2.3 Examples with structures (a) Acid Dyes- Orange II, (b) Basic Dyes-methyl violet, Victoria Blue B (c) Direct cotton Dyes- Benzofast Yellow 5GL (d) Azoic Dyes-Diazo components; Fast yellow G, Fast Orange R. Coupling components. Naphthol AS, Naphthol ASG (e) Mordant Dyes-Erichrome Black A, Alizarin. (f) Vat Dyes-Indanthrene brown RRD, Indanthrene Red 5GK. (g) Sulphur Dyes- Sulphur Black T (no structure) (h) Disperse Dyes-Celliton Fast brown 3R, perlon fastblue FFR
(i) Reactive Dye scibacron Brillant Red B, procion briilant Blue HB.

Unit 3 Considerations in Dye Design **(06 Hours)**

3.1 Dye -substrate affinity
3.2 Dyes for polyesters
3.3 Dyes for polyamides and proteins
3.4 Dyes for cationic polymers
3.5 Dyes for cellulosic polymers
3.6 Toxicological consideration
3.7 Structure -Property Relationship.

Unit 4 General Theory of Dyeing **(06 Hours)**

4.1 Introduction of Dyeing
4.2 Role of water
4.3 Role of electrolytes
4.4 High temperature the Dye Liquor
4.5 High temperature Dyeing
4.6 Dye auxiliaries compounds
4.6.1 Swelling agents
4.6.2 Levelling agents
4.7 Scouring after dyeing

Unit 5 Basic Operations in Dyeing Process **(08 Hours)**

5.1 Preparation of the fibres
5.2 Preparation of the dyebath, Application of the dyebath and finishing
5.3 Various methods of dyeing: Direct dyeing, Vat dyeing, Mordant dyeing, Disperse dyeing and Formation of dye on the fibre
5.4 Dyeing of wool with the acid dyes
5.5 Dyeing with the reactive dyes

Unit 6 Non Textile Uses of Dyes **(06 Hours)**

6.1 Biological staining agents Methylene blue, Crystal violet
6.2 Dyes as therapeutics: Mercurochrome, Acriflavine, Crystal violet, Prontosil
6.3 Dyes used in food and cosmetics
6.4 Paper and Leather Dyes
6.7 Miscellaneous Dyes: Hair dyes, Laser dyes, Indicators, Security inks

Unit 7 Pigments **(10 Hours)**

7.1 Introduction
7.2 Difference between Dyes and Pigments
7.3 Classification of pigments
7.4 Application of pigments
7.5 Raw materials for organic pigments
7.6 General methods of processing and synthesis of inorganic pigments: Crushing and grinding, vaporization, co precipitation, filtration, drying, flushing, calcinations/roasting, vapour phase oxidation etc.

Unit 8 Smart Dyes **(10 Hours)**

8.1 Introduction and types of Chromism
8.2 Application of smart and functional Dyes in Textiles
8.2.1 Electrochromic dyes
8.2.2 Thermochromic dyes
8.2.3 Photochromic dyes
8.2.4 Chemochromic dyes
8.2.5 Solvatochromic dyes
8.2.6 Mechano chromic dyes

Reference Books

1.Color Chemistry, 3rd Edition, Heinrich Zollinger, Wiley – VCH, 2003.
2. Organic Chemistry and Application Properties, John Shore, Society of Dyers &Colourists; 2nd Edition, 2002.
3. The Chemistry of Synthetic dyes, K. Venkataraman, 1971, Academic Press.
4. Industrial Inorganic Pigments, Gunter Buxbaum, 1st Edition, 2005, Wiley-VCH.
5. Industrial Organic Pigments: Production, Properties, Applications, 3rd Edition, 2006.
6. Application Properties of Pigments, A. Karnik, 1st Edition, 1999.
7. Chemistry of Synthetic Dyes and Pigments, Lubs H. A., Robert E. Krieger Publishing Company, New York, 1977.
8. Chemistry of Synthetic Dyes – Vol I, Venkataraman, K., 1952, Academic Press.
9. Chemistry of Synthetic Dyes – Vol III, Venkataraman, K., 1972, Academic Press.
10. Colour and Chemical Constitution of Organic Dyes, Griffiths J., 1976, Academic Press.
11. Quantum Chemistry, Chandra A. K., 1979, Tata McGraw Hill.
12. Color Chemistry –Synthesis, Properties and Applications of Dyes and Pigments, Zollinger H., 2nd Edition, 1991, Weinheim – VCH.