

**SARDAR PATEL UNIVERSITY
VALLABH VIDYANAGAR**



**SYLLABUS EFFECTIVE FROM: 2018-19
M.Sc. CHEMISTRY
SEMESTER-III
ORGANIC CHEMISTRY**

(Total 650 marks)

Course Code	Course Title	Hours per week	Internal Marks	External Marks	Total Marks
PS03CORC21	Organic Spectroscopy	4 hrs	30	70	100
PS03CORC22	Disconnection Approach	4 hrs	30	70	100
PS03CORC23	Heterocyclic Chemistry	4 hrs	30	70	100
PS03EORC21-22	Any One	4 hrs	30	70	100
PS03CORC24	Practicals OR	8 hrs	30	70	100
PS03CORC25	Project Work	8 hrs	30	70	100
PS03CORC26	Practicals OR	8 hrs	30	70	100
PS03CORC27	Project Work	8 hrs	30	70	100
PS03CORC28	Comprehensive Viva	1 hrs	-	50	50
Total Marks					650

* **Project work** (as optional) in place of practicals; to be offered to some of the students, based on their merit, interest and placement with the teachers (Marks : 200). The project shall have to be carried out under the allotted teacher(s) and a dissertation shall be submitted and will be assessed for internal (60 marks) and external (140 marks), in the usual manner.

Paper Code: PS03CORC21		Total Credit: 4
Title of Paper: Organic Spectroscopy		
Unit	Description in detail	Weightage
1	<p>UV Spectroscopy: Theory and principles of electronic transition and UV absorption; chromophores and auxochromes; Woodward-Fieser rules for dienes and enones; characteristic absorptions in alkenes and alkynes, alcohols, ethers, amines, carbonyl compounds, Characteristic absorptions in aromatic compounds; Factors influencing λ_{max}, effects of conjugation, effect of solvent; Differentiation of compounds/ isomers by UV</p> <p>Infrared Spectroscopy: Theory and principles; molecular vibrations; calculations of vibrational frequencies; Factors influencing IR frequency; characteristic group absorptions in hydrocarbons, aromatic compounds, alcohol and phenols, ethers, carbonyl compounds, amines, nitriles, nitro compounds,</p>	25%

	carboxylic acids and halide, Differentiation of compounds/isomers by IR	
2	<p>PMR Spectroscopy: Proton resonance condition, Various aspects of PMR spectra–(1) Number of signals, (2) Position of signals: chemical shifts, shielding and deshielding, (3) Splitting of the signals (spin-spin coupling), coupling constants – vicinal, geminal, long range and virtual couplings, (4) Intensity of signal (Peak area or integration); factors affecting chemical shifts, paramagnetic and diamagnetic anisotropy; Pople notation and spin assignments; chemical shift equivalence and magnetic equivalence; first order and second order spectra, complex PMR spectra; simplification of the complex PMR spectra- (1) Increasing field strength (high resolution spectra), (2) Use of shift reagents, (3) Spin-spin decoupling (Double resonance), (4) Proton exchange, (5) Deuterium exchange, (6) Nuclear Overhauser Effect (NOE); Differentiation of compounds/ isomers by PMR; To identify structure from PMR data</p>	25%
3	<p>¹³C-NMR Spectroscopy: Difficulties and solution for recording ¹³C-NMR spectra; recording of ¹³C-NMR spectra – scale, solvents, solvent signals and their positions, multiplicity, ¹³C-¹H coupling constant; proton coupled and decoupled ¹³C spectra, broad band decoupling, off resonance technique; Chemical shifts in ¹³C spectra – chemical shift calculation for alkanes, alkenes and alkynes, chemical shift calculation in internal and terminal substituted compounds, aromatic compounds; To identify structure from ¹³C NMR data; Use of ¹³C spectra in differentiating compounds/isomers; ¹³C-DEPT Spectra – Differentiation in Primary, Secondary and Tertiary Carbons by DEPT–45°, DEPT–90°, DEPT–135° spectra; 2D NMR Spectroscopy: Theory and Principles Of 2D NMR Spectroscopy (COSY); To interpret or to draw HOMCOR (1H-1H COSY, DQF-COSY, INADEQUATE),HETCOR (¹³C-¹H COSY, ¹H-¹³C COSY i.e. HMQC, HMBC), NOESY and TOCSY spectra. Introduction to NMR of nuclei other than proton and carbon.</p>	25%
4	<p>Mass Spectroscopy: Theory and principles of mass spectroscopy; Instrumentation; low and high resolution mass spectra; Ionization techniques – Electron Impact (EI) ionization, Chemical Ionization (CI), Field Desorption (FD), Fast Atom Bombardment (FAB), Electrospray Ionization (ESI) and Matrix Assisted Laser Desorption/Ionization (MALDI); Determination of molecular weight and molecular formula, nitrogen rule, detection of molecular ion peak, metastable ion peak; Fragmentations – rules governing the fragmentations, McLafferty rearrangement; Interpretation of mass spectra of different class of compounds – saturated and unsaturated hydrocarbons, aromatic hydrocarbons, alcohols, ethers, ketones, aldehydes, carboxylic acids, amines, amides, compounds containing halogens; To write possible fragmentation for given</p>	25%

	compound; To identify structure from mass spectral data; To identify structure from combined spectral data.	
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Basic Text & Reference Books:-

1. Spectroscopic Identification of Organic Compounds, R. M. Silverstein and F. X. Webster, 6th edition (John Wiley & Sons)
2. Introduction to Spectroscopy, D. L. Pavia, G. M. Lampman and G. S. Kriz, 3rd edition (Thomson Brooks/Cole)
3. Spectroscopic Methods in Organic Chemistry, D. H. Williams and I. Fleming, 4th edition (Mcgraw – Hill Book Company)
4. Organic Spectroscopy, William Kemp, 3rd edition (Palgrave)
5. Organic Spectroscopy – Principles and Applications, Jag Mohan, 2nd edition (Narosa Publishing House)
6. Spectroscopy of Organic Compounds, P. S. Kalsi, 5th edition (New Age International Publishers)
7. Elementary Organic Spectroscopy: Principles and Chemical applications (revised edition), Y. R. Sharma (S. Chand Publishing)

Paper Code: PS03CORC22		Total Credit: 4
Title of Paper: Disconnection Approach		
Unit	Description in detail	Weightage
1	Introduction and definition of disconnection, various terminology used in disconnection. One and two group disconnection, disconnection and synthesis of alcohols, olefins, simple ketones, acids and its derivatives, disconnections in 1,3- dioxxygenated skeletons, preparation of β -hydroxy carbonyl compounds, α,β - unsaturated carbonyl compounds, 1,3-dicarbonyls, 1,5-dicarbonyls and use of Mannich reaction	25%
2	Illogical Two group disconnection: Disconnection and synthesis of α -hydroxy carbonyl compounds, 1,2-diols, 1,4- and 1,6- dicarbonyl compounds. Disconnections based on Diels-Alder reaction and its use in organic synthesis. Functional group analysis: Strategy of saturated hydrocarbon synthesis, functional group addition to intermediates.	25%
3	Disconnection and synthesis of acyclic and cyclic hetero compounds: Synthesis of ethers, amines, nitrogen, oxygen and sulphur containing five and six membered heterocycles. Synthesis of small ring compounds: Special method for small rings preparations, synthesis of 3 and 4 membered ring compounds. Use of ketenes in organic synthesis, Radical reactions in organic synthesis.	25%
4	Protecting groups: Protection of organic functional groups, protecting reagents and removal of protecting groups. Protection of amine: Via N-benzylamine formation, amide formation, carbamate formation. Protection of alcohol: Via alkyl ether formation, benzyl ether formation, trityl ether formation, silyl ether formation, acetal formation, methoxyl methyl ether formation, ester formation. Protection of 1,2- and 1,3-diols, Protection of acid via ester formation, Protection of aldehyde via acetal formation, Protection of ketone via ketal formation. Fragmentation Reactions: Grob fragmentation: Polarization of C-C bond, fragmentation controlled by stereochemistry, ring expansion by fragmentation. Eschenmoser Fragmentation: Controlling double bond using fragmentation. Synthesis of some complex molecules: Synthesis of Mesoporphyrin – IX and Cephalosporin C. Synthesis of Nootkatone via Fragmentation of three membered, four membered and six membered ring	25%

Basic Text & Reference Books:-

1. Designing Organic Synthesis – A Programmed Introduction to the Synthons Approach, Stuart Warren, John Wiley & Sons (1994).

2. Organic Synthesis: The disconnection approach, Stuart Warren, John Wiley & Sons (1994).
3. Selected Organic Synthesis, Ian Fleming, John Wiley & Sons (1977).
4. Organic Chemistry, 2nd edition by Jonathan Clayden, Nick Greeves & Stuart Warren, Oxford University Press.
5. Modern Methods of Organic Synthesis, 4th edition by W. Carruthers & Iain Coldham, Cambridge University Press.
6. Modern Organic Synthesis: An introduction by George S. Zweifel & Michael H. Nantz, W. H. Freeman & Company.
7. Greene's Protective Groups in Organic Synthesis, 4th edition, by P. G. M. Wuts and T. W. Greene, Wiley Interscience.

Paper Code: PS03CORC23		Total Credit: 4
Title of Paper: Heterocyclic Chemistry		
Unit	Description in detail	Weightage
1	<p>Hantzsch-Widman nomenclature systems,</p> <p>Indole: Biological importance of indole derivatives, Reactions: protonation, nitration, sulphonation, halogenation, acylation, alkylation, reaction with aldehydes and ketones, reaction of α,β-unsaturated ketones, nitriles and nitro compounds. Mannich reaction, reaction with oxidizing agents, reaction with nucleophilic reagents, reaction with N-metallatedindole. Reaction with reducing agents. Reaction with carbenes, electrophilic and photochemical reactions. Reaction of indolyl C-X compounds, electrophilic substitution reactions of substituted indoles.</p> <p>Synthesis: Fischer-indole synthesis (From phenyl hydrazone of aldehyde and ketone), Grandberg synthesis, Reissert synthesis, Modelung synthesis.</p> <p>Reactions and synthesis of benzo[b]thiophene and benzo[b]furan.</p>	25%
2	<p>Reactions and Synthesis of bicyclic heterocycles</p> <p>Quinoline / Isoquinoline</p> <p>Reactions: Substitution of carbon: proton exchange, nitration, sulphonation, halogenation, reactions with nucleophilic reagents with hydride transfer: alkylation, arylation, amination, hydroxylation. Nucleophilic substitutions with displacement of halide, metal halogen exchange, reactions with reducing agents, Grignard reaction. Electrophilic substitution reactions of substituted quinoline and isoquinoline. Reissert reaction. Reactions of quinolone-N-oxide and isoquinoline-N-oxide with acid chloride, POCl_3, SOCl_2, diethylcyanophosphonate.</p> <p>Synthesis of quinoline: Skraup synthesis, Combes synthesis, Conrad Limpach Knorr synthesis, Pfitzinger synthesis, Pomeranz-Fritsch synthesis.</p> <p>Synthesis of isoquinoline: Bischer-Napieralski synthesis</p> <p>Heterocyclic system containing two nitrogen atoms: Cinnoline, Quinoxaline, Phthalazine: Synthesis and its reactions</p>	25%
3	<p>Reactions and synthesis of six membered heterocycles containing nitrogen.</p> <p>Pyridine: Brief introduction, electrophilic substitution of substituted pyridines.</p> <p>Pyridine-N-oxide: Reactivity, electrophilic addition and substitution, nucleophilic addition and substitution reactions, Rearrangement, Electrophilic substitution reaction of substituted Pyridine-N-oxide, Synthesis of PNO.</p>	25%

	<p>Diazines: Introduction, Reactions: Addition at nitrogen, Substitution at carbon, oxidizing agents, nucleophilic agents, replacement of hydrogen, replacement of good leaving group, Reaction of oxydiazine, Anrorc mechanism. Synthesis of diazines.</p> <p>Triazine: Introduction, reactions and synthesis.</p> <p>Tetrazine: Introduction, reactions and synthesis.</p>	
4	<p>Reactions and synthesis of oxygen containing heterocycle: Typical reactivity of pyrilium and benzopyrilium ions, pyrones and benzopyrones.</p> <p>Pyrilium salts: Reactions: electrophilic reagents, nucleophilic reagents and reducing agent. Synthesis from 1,5-dicarbonyl compounds, 1,3-dicarbonyl compounds and ketones. Alkene acylation.</p> <p>2- and 4-Pyrone: Reactions: Electrophilic addition and substitution, nucleophilic reagents, cycloaddition reactions. Synthesis of 2- and 4-Pyrones.</p> <p>Benzopyrilium salt: Reaction with nucleophilic reagents, reducing and oxidizing agents, Synthesis from phenols and 1,3-dicarbonyl compounds, ortho-hydroxybenzaldehydes and ketones.</p> <p>Benzopyranones: Reaction with electrophilic reagents, nucleophilic reagents, oxidizing and reducing agents, cycloaddition and photochemical reactions. Synthesis of Coumarin: Phenols and 1,3-ketoesters, from o-hydroxybenzaldehydes and anhydrides. Synthesis of Chromone: From o-hydroxy acyl benzenes and esters. Isocoumarin synthesis.</p> <p>Azoles: Typical reaction of 1,2- and 1,3-azoles.</p> <p>1,3-Azoles: Reactions: electrophilic reagents, Addition at nitrogen, substitution at carbon, nucleophilic reagents, C-metalled-1,3-azoles, alkyl-1,3-azoles. Synthesis.</p> <p>1,2-Azoles: Reactions: electrophilic reagents, Addition at nitrogen, substitution at carbon, nucleophilic and reducing reagents. Synthesis.</p>	25%

Basic Text & Reference Books:-

1. Heterocyclic Chemistry, 4th Edition by J. A. Joule & K. Mills, Published by Chapman & Hall (1995)
2. Principles of modern heterocyclic chemistry, Edited by Leo A. Paquette, Published by Pearson Benjamin Cummings (1968)
3. Heterocyclic Chemistry, 3rd Edition by Thomas L. Gilchrist, Published by Prentice Hall (1997)
4. The Structure & Reactions of Heterocyclic Compounds, Edited by Michael Henry Palmer, Published by Edward Arnold (1967)
5. Heterocyclic chemistry by V. K. Ahluwalia, Narosa publishing house.

Paper Code: PS03EORC21		Total Credit:
Title of Paper: Selected Topics in Organic Chemistry		4
Unit	Description in detail	Weightage
1	Dyes: Brief introduction to fundamentals of dyes; Classification of dyes-based on structure and applications; Non textile dyes-Leather, food, hair, ink, photographic, indicator, NIR, Indigo dyes	25%
2	Pigments: Organic and Inorganic pigments-Introduction, classification, characteristics and applications. Organic pigments- Synthesis and evaluation. FBA-Characteristics, classification, synthesis and applications. Colour photography, LCD	25%
3	Pericyclic Reactions-I: General introduction, Theories of pericyclic reactions: FMO, Woodward-Hoffmann rules, Huckel-Mobius rules. Electrocyclic reactions: Ring opening and closing reactions of $4n$ and $4n+2$ system; cation (Nazarov reaction) and anion type molecules; small ring opening. Sigmatropic reactions: [1, n]; [2, 3] –SeO ₂ , Sommellet-Haouser, Wittig, Mislow Evan's rearrangements; [3, 3]- Cope, Claisen, Claisen-Cope, Aza-Cope; [5, 5].	25%
4	Pericyclic Reactions-II: Theories of pericyclic reactions: FMO, Woodward-Hoffmann rules, Huckel-Mobius rules. Cycloadditions: [2+2] thermal and photochemical; [4+2]-Diels-Alder reactions, diene and dinophile nature; Inter, intra and hetero cycloaddition reaction with region and stereoselectivity. [3+2]-dipolar cycloaddition, introduction of different dipoles, their reactions dipolarophiles (inter, intra) Cycloadditions reactions of more than six π electrons. Group transfer reactions: Ene reactions, diimide (N ₂ H ₂), syn β -elimination.	25%

Basic Text & Reference Books:-

1. Colour Chemistry : Synthesis, Properties and applications of Organic dyes and pigments, A. T. Peters, H. S. Freeman
2. The Chemistry of Synthetic dyes and pigments, by H. A. Lubs, Reinhold Publication (1955)
3. The Chemistry of Synthetic dyes, Volume I to IX, Edited by K. Venkataraman, Academic Press (1971)
4. The production and applications of fluorescent Brighteing Agents, Milos Zahradnik, John Wiley & Sons. 1982

5. Synthetic dyes, Gurdeep R. Chatwal, 4th revised and enlarged edition, Himalaya Publishing House
6. Handbook of synthetic dyes and pigments, Vol. – 2 (Intermediates), 2nd edition, K. M. Shah, Multi-tech publishing co. Mumbai
7. Handbook of synthetic dyes and pigments, Vol. – 3 (Pigments), 2nd edition, K. M. Shah, Multi-tech publishing co. Mumbai
8. Aspects of organic photochemistry, William M. Horspool, Academic Press
9. Frontier orbitals and organic chemical reactions, Ian Fleming,
10. Molecular Orbitals and Organic Chemical Reactions, Student Edition, Ian Fleming, (2010), Wiley
11. Pericyclic reactions, Ian Fleming, oxford
12. Advance organic chemistry: part A & B, Carey and Sundberg
13. Photochemistry and pericyclic reactions, Jagdamba Singh, Jaya Singh,
14. Modern methods of organic synthesis, 4th edition, W. Carruthers , Iain Coldham, Cambridge university press,
15. Organic chemistry, 2nd edition, J. Clayden, N. Greeves, S. Warren, Oxford university press
16. Organic chemistry, 7th edition, R. T. Morrison, R. N. Boyd, S. K. Bhattacharjee, Pearson

Paper Code: PS03EORC22		Total Credit: 4
Title of Paper: Occupational Practices		
Unit	Description in detail	Weightage
1	Intellectual Property Rights: Introduction to intellectual properties; Need for protection of intellectual properties; Industrial property: patents, trademark, industrial design and geographical indications; Copyright and neighbouring rights; IPR legislations in India, World IP organizations and treaties; Indian patent act; Patentability; Patent applications; Patent registration and filing; Patent cooperation treaty.	25%
2	Validation of analytical methods and processes: General principles of analytical method validation, parameters for method validation: specificity, selectivity, precision, accuracy, linearity and calibration curve, Range, Limit of detection and quantification, Robustness. Introduction to process validation; Regulatory basis for process validation; Pharmaceutical process validation; FDA guidelines; cGMP and GLP: cGMP guidelines viz. ICH/WHO/USFDA/EDQM/ Schedule M/NDA/AMDA.	25%
3	Hazards: Classification Hazardous chemical, transportation of Hazardous chemicals, Storage, Handling and control measures for hazardous chemicals. Hazards and controls in Unit process and Unit Operations. Hazards – fire, mechanical, electrical, chemical and pharmaceutical, Monitoring & prevention systems, industrial effluent testing & treatment. Control of environmental pollution.	25%
4	Concept of Industrial Safety: Accidents investigation and Analysis, Statutory provisions, Types of chemical hazards and control, control techniques, process flow chart and its importance for safety inspection, interpretation, use and training of MSDS, UN, HAZCHEM. Safety in chemical industry: General introduction, type of chemical hazards, Safety and risk phrases, Storage hazards and control, Prevention of overflow-pressure-temperature and process flow, Types of guards and valves for the vessel, its inlet and out let, need of remote and auto control valves, Process hazards and controls.	25%

Basic Text & Reference Books:-

1. Intellectual Property Rights under WTO: Tasks Before India, Author: T. Rammappa – New Delhi, Wheeler Publishing, 2000.
2. Intellectual Property Rights: Text & Cases; Author: Dr. S. Balasubhranian Dr. R. Radhakrishnan, Publisher: Excel Books N Delhi, ISBN: 8174466096, ISBN-13: 9788174466099.
3. How to Practice GMPs, Author: P.P. Sharma, Vandana Publications, Agra
4. Pharmaceutical Process Validation, Author: Ira R. Berry and Robert Nash, Publisher: Marcel Decker Inc. (2nd edition).

5. Accident prevention manual for industrial operations, National safety council, Chicago, 10th edition.
6. Safety and Accident prevention in chemical operation, 2 nd edition, Howard H.
7. Handbook of occupational safety and Health by S. Lawrence.
8. MSDS – your guide to chemical safety
9. Engineering design for control of work place hazards, A. Richard
10. Safety managers Handbook, J. J. Keller and Associates Inc, USA.
11. Supervising safety for hazardous Processes, Dr. K. U. Mistry, Safety Health and Environment Association, 1st edition.
12. Fundamental of Industrial safety and health by Dr. K. U. Mistry

Paper Code: PS03CORC24	Total Credit: 4
Title of Paper: Practical in Organic Chemistry	

Description in detail	Weightage (%)
Separation and identification of Ternary Organic Mixture and Spectral Exercise	100%

A. Separation and identification of Ternary Organic Mixture

Minimum two (02) mixtures should be given from each of the following type

1. Solid + Solid + Solid
2. Solid + Solid + Solid (one soluble)
3. Solid + Solid + Liquid
4. Solid + Liquid + Liquid
5. Liquid + Liquid + Liquid

B. Spectral Exercise

- Structure interpretation of organic compounds from spectral data

Basic Text & Reference Books:-

1. Vogel's Textbook of practical organic chemistry, 5th edition, B. S. Furniss, A. J. Hannaford, P. W. G. Smith, A. R. Tatchell (Pearson Education)
2. Comprehensive practical organic chemistry: Qualitative analysis, V. K. Ahluwalia, SunitaDhingra (Universities Press)
3. Organic structures from spectra, 5th edition, L. D. Field, S. Sternhell, J. R. Kalman (Wiley: A John Wiley & Sons Ltd publication)
4. Elementary Organic Spectroscopy: Principles and Chemical applications (revised edition), Y. R. Sharma (S. Chand Publishing)

Paper Code: PS03CORC26	Total Credit: 4
Title of Paper: Practical in Organic Chemistry	

Description in detail	Weightage (%)
Synthesis and Application of Dyes & Intermediates	100%

- A. Synthesis of Azo dye (including azoic dye, disperse azo dye and acid azo dye) and its dyeing on various fiber. Dyeing of Indigo (Vat dyeing). Also some intermediate use for above dyeing.
- B. Synthesis of dyes, pigments and intermediate
1. o-Cresolphthalein
 2. Phenolphthalein
 3. Fluorescein and its methylation
 4. Quinizarin
 5. 1, 5-Dinitroanthraquinone
 6. Bisazo acid dye
 7. Acetoacetanilide pigment
 8. Indigo from phenylglycin-o-carboxylic acid and its dyeing (Vat dyeing)

Basic Text & Reference Books:-

1. Vogel's Textbook of practical organic chemistry, 5th edition, B. S. Furniss, A. J. Hannaford, P. W. G. Smith, A. R. Tatchell (Pearson Education)
2. Comprehensive practical organic chemistry: Preparation and Quantitative analysis, V. K. Ahluwalia, Renu Aggarwal (Universities Press)

OR

PS03CORC25 and PS03CORC27:

* **Project work** (as optional) in place of practicals; to be offered to some of the students, based on their merit, interest and placement with the teachers (Marks : 200). The project shall have to be carried out under the allotted teacher(s) and a dissertation shall be submitted and will be assessed for internal (60 marks) and external (140 marks), in the usual manner.

Paper Code: PS03CORC28	Total Credit: 1
Title of Paper: Comprehensive Viva	

Description in detail	Weightage (%)
Viva Voce From the Subjects Studied in Semester - III	100%