



MANAV RACHNA UNIVERSITY

FACULTY OF APPLIED SCIENCES DEPARTMENT OF CHEMISTRY

PROGRAM STRUCTURE & DETAILED SYLLABUS

**M.Sc. Chemistry
BATCH: 2016-2018**



MANAV RACHNA UNIVERSITY

DEPARTMENT OF CHEMISTRY

M.SC (CHP01)

SEMESTER - 1

| S.No. | SUBJECT CODES | SUBJECT NAME | OFFERING DEPARTMENT | *COURSE NATURE (Hard/Soft/Workshop/NTCC) | COURSE TYPE (Core/Elective / University Compulsory) | L | T | P | O | NO. OF CONTACT HOURS PER WEEK | NO. OF CREDITS |
|--|---------------|---|---------------------|--|---|-----------|----------|-----------|----------|-------------------------------|----------------|
| 1 | CHH501 | INORGANIC CHEMISTRY-I | CH | HARD | CORE | 4 | 0 | 0 | 0 | 4 | 4 |
| 2 | CHH502 | ORGANIC CHEMISTRY-I | CH | HARD | CORE | 4 | 0 | 0 | 0 | 4 | 4 |
| 3 | CHH503 | PHYSICAL CHEMISTRY-I | CH | HARD | CORE | 4 | 0 | 0 | 0 | 4 | 4 |
| 4 | CHH504 | ANALYTICAL TECHNIQUES and SPECTROSCOPY- I | CH | HARD | CORE | 4 | 0 | 0 | 0 | 4 | 4 |
| 5 | CHH505 | LABORATORY WORK-I | CH | HARD | CORE | 0 | 0 | 8 | 0 | 8 | 4 |
| 6 | CHW506 | WORKSHOP | CH | WORKSHOP | CORE | 0 | 0 | 3 | 0 | 3 | 2 |
| 7 | PHS501 | RESEARCH METHODOLOGY | PH | SOFT | CORE | 1 | 0 | 2 | 0 | 3 | 2 |
| TOTAL (L-T-P-O/CONTACT HOURS/CREDITS) | | | | | | 17 | 0 | 13 | 0 | 30 | 24 |

SEMESTER - 2

| | SUBJECT CODES | SUBJECT NAME | OFFERING DEPARTMENT | *COURSE NATURE (Hard/Soft/Workshop/NTCC) | COURSE TYPE (Core/Elective / University Compulsory) | L | T | P | O | NO. OF CONTACT HOURS PER WEEK | NO. OF CREDITS | |
|--|---------------|---|---------------------|--|---|-----------|----------|-----------|----------|-------------------------------|----------------|--|
| 8 | CHH508 | INORGANIC CHEMISTRY-II | CH | HARD | CORE | 4 | 0 | 0 | 0 | 4 | 4 | |
| 9 | CHH509 | ORGANIC CHEMISTRY-II | CH | HARD | CORE | 4 | 0 | 0 | 0 | 4 | 4 | |
| 10 | CHH510 | PHYSICAL CHEMISTRY-II | CH | HARD | CORE | 4 | 0 | 0 | 0 | 4 | 4 | |
| 11 | CHH511 | ANALYTICAL TECHNIQUES and SPECTROSCOPY- II | CH | HARD | CORE | 4 | 0 | 0 | 0 | 4 | 4 | |
| 12 | CHH512 | LABORATORY WORK-II | CH | HARD | CORE | 0 | 0 | 8 | 0 | 8 | 4 | |
| 13 | CHW513 | WORKSHOP | CH | WORKSHOP | CORE | 0 | 0 | 3 | 0 | 3 | 2 | |
| 14 | MES515 | RESEARCH PAPER WRITING | ME | SOFT | CORE | 1 | 0 | 2 | 0 | 3 | 2 | |
| TOTAL (L-T-P-O/CONTACT HOURS/CREDITS) | | | | | | 17 | 0 | 13 | 0 | 30 | 24 | |
| 15 | CHW514 | Post 2nd Semester Summer Training 3 credit | | | | | | | | | | |

| SEMESTER - 3 | | | | | | | | | | | |
|--|--------------------------|--|--|---|-----------|----------|-----------|----------|-------------------------------|----------------|---|
| SUBJECT CODES | SUBJECT NAME | OFFERING DEPARTMENT | *COURSE NATURE (Hard/Soft/Workshop/NTCC) | COURSE TYPE (Core/Elective / University Compulsory) | L | T | P | O | NO. OF CONTACT HOURS PER WEEK | NO. OF CREDITS | |
| 16 | CHH615 | Conformational Analysis, Asymmetric Synthesis and Biomolecules | CH | HARD | CORE | 4 | 0 | 0 | 0 | 4 | 4 |
| 17 | CHH616 | Modern Organic Synthetic Techniques & Stereochemistry | CH | HARD | CORE | 4 | 0 | 0 | 0 | 4 | 4 |
| 18 | CHH617 CHH618 | ELECTIVE-I (A) Orgnaometallic Chemistry of Transition Metals & Bio-inorganic Chemistry (B) Drug Design | CH | HARD | ELECTIVE | 4 | 0 | 0 | 0 | 4 | 4 |
| 19 | CHH619 | Photochemistry and pericyclic reaction | CH | HARD | CORE | 4 | 0 | 0 | 0 | 4 | 4 |
| 20 | CHH620 | LABORATORY WORK-III | CH | HARD | CORE | 0 | 0 | 6 | 0 | 6 | 3 |
| 21 | CHH621 | LABORATORY WORK-IV | CH | HARD | CORE | 0 | 0 | 6 | 0 | 6 | 3 |
| 22 | CHN622 | SEMINAR | CH | HARD | CORE | 0 | 0 | 0 | 2 | 2 | 2 |
| TOTAL (L-T-P-O/CONTACT HOURS/CREDITS) | | | | | 16 | 0 | 12 | 2 | 30 | 24 | |
| SEMESTER - 4 | | | | | | | | | | | |
| SUBJECT CODES | SUBJECT NAME | OFFERING DEPARTMENT | *COURSE NATURE (Hard/Soft/Workshop/NTCC) | COURSE TYPE (Core/Elective / University Compulsory) | L | T | P | O | NO. OF CONTACT HOURS PER WEEK | NO. OF CREDITS | |
| 23 | CHH623 | Advanced Hetrocyclic Chemistry | CH | HARD | CORE | 4 | 0 | 0 | 0 | 4 | 4 |
| 24 | CHH624 | Chemistry of Natural Products | CH | HARD | CORE | 4 | 0 | 0 | 0 | 4 | 4 |
| 25 | (A) CHH625 (B) CHH626 | ELECTIVE-II : (A) BIOORGANIC CHEMISTRY (B) GROUP THEORY AND ITS APPLICATIONS | CH | HARD | ELECTIVE | 4 | 0 | 0 | 0 | 4 | 4 |
| 26 | CHH627 | LABORATORY WORK-V | CH | HARD | CORE | 0 | 0 | 6 | 0 | 6 | 3 |
| 27 | CHN628 | Project Work | CH | HARD | CORE | 0 | 0 | 0 | 6 | 6 | 6 |
| TOTAL (L-T-P-O/CONTACT HOURS/CREDITS) | | | | | 12 | 0 | 6 | 6 | 24 | 21 | |



MANAV RACHNA UNIVERSITY

FACULTY: FACULTY OF APPLIED SCIENCES

PROGRAM: M.Sc. CHEMISTRY

PROGRAM CODE: CHP01

SYLLABUS: SCHEME A



MANAV RACHNA UNIVERSITY
FACULTY OF APPLIED SCIENCES
DEPARTMENT OF CHEMISTRY
M.SC. (2016-18)
SYLLABUS & SCHEME
(CHP01) SEMSETER I

| COURSE CODES | COURSE NAME | COURSE TYPE | COURSE NATURE | PERIODS | | | | NO. OF CONTACT HOURS PER WEEK | CREDITS |
|--------------|-----------------------|---|---------------------------------|---------|---|---|---|-------------------------------|---------|
| | | Core(Departmental/Allied)/ Elective (Departmental/ Open) / University Compulsory | Hard/Soft/ Workshop/ NTCC | L | T | P | O | | |
| CHH501-T | INORGANIC CHEMISTRY-I | CORE(Departmental) | HARD | 4 | 0 | 0 | 0 | 4 | 4 |
| CHH502-T | ORGANIC CHEMISTRY-I | CORE(Departmental) | HARD | 4 | 0 | 0 | 0 | 4 | 4 |
| CHH503-T | PHYSICAL CHEMISTRY-I | CORE(Departmental) | HARD | 4 | 0 | 0 | 0 | 4 | 4 |
| CHH504-T | ANALYTICAL CHEMISTRY | CORE(Departmental) | HARD | 4 | 0 | 0 | 0 | 4 | 4 |
| CHH505-P | LABORATORY WORK-I | CORE(Departmental) | HARD | 0 | 0 | 8 | 0 | 8 | 4 |
| CHW506 | WORKSHOP | CORE(Departmental) | WORKSHOP | 0 | 0 | 3 | 0 | 3 | 2 |
| PHS-501 | RESEARCH METHODOLOGY | CORE(Allied) | HARD | 1 | 0 | 2 | 0 | 3 | 2 |

SEMESTER II

| COURSE CODES | COURSE NAME | COURSE TYPE | COURSE NATURE | PERIODS | | | | NO. OF CONTACT HOURS PER WEEK | CREDITS |
|--------------|------------------------|--|---------------------------------|---------|---|---|---|-------------------------------|---------|
| | | Core(Departmental/Allied)/ Elective (Departmental/ Open) / University Compulsory | Hard/Soft/ Workshop/ NTCC | | | | | | |
| CHH508-T | INORGANIC CHEMISTRY-II | CORE(Departmental) | HARD | 4 | 0 | 0 | 0 | 4 | 4 |
| CHH509-T | ORGANIC CHEMISTRY-II | CORE(Departmental) | HARD | 4 | 0 | 0 | 0 | 4 | 4 |
| CHH510-T | PHYSICAL CHEMISTRY-II | CORE(Departmental) | HARD | 4 | 0 | 0 | 0 | 4 | 4 |
| CHH511-T | SPECTROSCOPY | CORE(Departmental) | HARD | 4 | 0 | 0 | 0 | 4 | 4 |
| CHH512-P | LABORATORY WORK-II | CORE(Departmental) | HARD | 0 | 0 | 8 | 0 | 8 | 4 |
| CHW513 | WORKSHOP | CORE(Departmental) | WORKSHOP | 0 | 0 | 3 | 0 | 3 | 2 |
| MES 515 | RESEARCH PAPER WRITING | CORE (Allied) | SOFT | 1 | 0 | 2 | 0 | 3 | 2 |
| CHW514 | SUMMER TRAINING | | | | | | | | 3 |

SEMSETER III

| COURSE CODES | COURSE NAME | COURSE TYPE | COURSE NATURE | PERIODS | | | | NO. OF CONTACT HOURS PER WEEK | CREDITS |
|----------------------|---|--------------------|---------------|---------|---|---|---|-------------------------------|---------|
| | | | | L | T | P | O | | |
| CHH615-T | CONFORMATIONAL ANALYSIS, ASYMMETRIC SYNTHESIS & BIOMOLECULES | Core(Departmental) | HARD | 4 | 0 | 0 | 0 | 4 | 4 |
| CHH616-T | MODERN ORGANIC SYNTHESIS (REAGENTS & SYNTHETIC TECHNIQUES) | Core(Departmental) | HARD | 4 | 0 | 0 | 0 | 4 | 4 |
| CHH617-T CHH618-T | ELECTIVE-I (A) BIOINORGANIC CHEMISTRY & ORGANOMETALLIC CHEMISTRY (B) DRUG DESIGN | Core(Departmental) | ELECTIVE | 4 | 0 | 0 | 0 | 4 | 4 |
| CHH619-T | PHOTOCHEMISTRY & PERICYCLIC REACTIONS | Core(Departmental) | HARD | 4 | 0 | 0 | 0 | 4 | 4 |
| CHH620-P | LABORATORY WORK-III | Core(Departmental) | HARD | 0 | 0 | 6 | 0 | 6 | 3 |
| CHH621-P | LABORATORY WORK-IV | Core(Departmental) | HARD | 0 | 0 | 6 | 0 | 6 | 3 |
| CHN622 | SEMINAR | Core(Departmental) | | 0 | 0 | 0 | 2 | 2 | 2 |

SEMSETER IV

| COURSE CODES | COURSE NAME | COURSE TYPE | COURSE NATURE | PERIODS | | | | NO. OF CONTACT HOURS PER WEEK | CREDITS |
|----------------------|--|---|-----------------------------|---------|---|---|---|-------------------------------|---------|
| | | Core(Departmental/Allied)/ Elective (Departmental/Open) / University Compulsory | Hard/Soft/Workshop/ NTCC | L | T | P | O | | |
| CHH623-T | ADVANCED HETEROCYCLIC CHEMISTRY | CORE(Departmental) | HARD | 4 | 0 | 0 | 0 | 4 | 4 |
| CHH624-T | CHEMISTRY OF NATURAL PRODUCTS | CORE(Departmental) | HARD | 4 | 0 | 0 | 0 | 4 | 4 |
| CHH625-T CHH626-T | ELECTIVE-II (A) BIOORGANIC CHEMISTRY(B) GROUP THEORY AND ITS APPLICATIONS | ELECTIVE(Departmental) | HARD | 4 | 0 | 0 | 0 | 4 | 4 |
| CHH627-P | LABORATORY WORK-V | CORE(Departmental) | HARD | 0 | 0 | 6 | 0 | 6 | 3 |
| CHN628 | PROJECT WORK | CORE(Departmental) | NTCC | 0 | 0 | 0 | 6 | 6 | 6 |

TOTAL CREDITS FOR SEMESTER I -IV

| S.No. | Semester | Credits |
|--|--|-----------|
| 1 | I | 24 |
| 2 | II | 24 |
| 3 | SUMMER TRAINING (POST 2 nd SEM) | 3 |
| 4 | III | 24 |
| 5 | IV | 21 |
| TOTAL CREDITS FOR M.Sc. CHEMISTRY PROGRAMME | | 96 |

SECTION WEIGHTAGE PARAMETERS

| Syllabus | Sections | Weightage |
|----------|--------------|-------------|
| | A | 25% |
| | B | 25% |
| | C | 25% |
| | D | 25% |
| | TOTAL | 100% |

DETAILED SYLLABUS
CHP01 –FIRST SEMESTER

| | |
|--------------------------|---|
| Course Title/Code | Inorganic Chemistry-I (CHH501-T) |
| Course Type | Core |
| Course Nature | Hard |
| L-T-P-O Structure | 4-0-0-0 |
| Objectives | To familiarize students with Metal-Ligand Bonding in Transition Metal Complexes To impart knowledge on Electronic Spectra of Transition Metal Complexes |
| Outcome | The students will be able to understand ML bonding in transition metal complexes. The students will be able to understand electronic spectra of transition metal complexes. The students will be able to understand VSEPR and HSAB theory |
| Prerequisites | B.Sc. with Chemistry as one of the Subject |

SECTION-A

METAL-LIGAND BONDING IN TRANSITION METAL COMPLEXES : Crystal field theory, Crystal field splitting diagrams in complexes; Spectrochemical and Nephelauxetic series; thermodynamic and structural effects; site selection in spinels, Jahn-Teller distortions; experimental evidence for metal-ligand orbital overlap; ligand field theory, molecular orbital theory of octahedral complexes.

SECTION-B

ELECTRONIC SPECTRA OF TRANSITION METAL COMPLEXES: Spectroscopic ground states; Orgel energy level and Tanabe-Sugano diagrams for transition metal complexes; Charge transfer spectra; electronic spectra of octahedral and tetrahedral complexes and calculation of ligand-field parameters.

SECTION-C

VSEPR THEORY: Valence Shell Electron Pair Repulsion Theory-stereochemical rules and explanation of the shapes of molecules and ions of non-transition elements with 2-7 valence shell electron pairs.

SECTION-D

HSAB Theory : Classification of acids and bases as hard and soft; HSAB principle, theoretical basis of hardness and softness; Lewis-acid base reactivity approximation; donor and acceptor numbers, E and C equation; applications of HSAB concept.

Books Recommended

1. J. E. Huheey, E. A. Keiter and R. L. Keiter; Inorganic Chemistry: Principles of Structure and Reactivity, Pearson Education, 2006.
2. P.W. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong; Shriver & Atkins: Inorganic Chemistry, 4th ed. Oxford University Press, 2006.
3. F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann; Advanced Inorganic Chemistry, 6th ed. Wiley, 1999.
4. R. C. Mehrotra and A. Singh, Organometallic Chemistry, A Unified Approach, New Age International, 2006.
5. Basic Organometallic Chemistry: Concepts, Syntheses and Applications of Transition metals, 2010, CRC Press and Universities Press.
6. J.D.Lee. Concise course in Inorganic Chemistry-

| | |
|--------------------------|---|
| Course Title | Organic Chemistry-I (CHH502-T) |
| Course Type | Core |
| Course Nature | Hard |
| L-T-P-O Structure | 4-0-0-0 |
| Objectives | To familiarize students with aromaticity and Effects of Structure on Reactivity To impart knowledge of Nucleophilic Substitution and reactivity effects of substrate structure |

| | |
|----------------------|--|
| Outcome | Students will be able to understand the concept of aromaticity and structure- reactivity correlation. Students will be able to grasp in depth knowledge of Nucleophilic and Electrophilic Substitution reactions. |
| Prerequisites | B.Sc. with Chemistry as one of the Subject |

| Syllabus | Sections | Weightage |
|----------|----------|-----------|
| | A | 25% |
| | B | 25% |
| | C | 25% |
| | D | 25% |
| | TOTAL | 100% |

SECTION-A

AROMATICITY: Benzenoid and non-benzenoid systems, anti-aromaticity, homoaromaticity, alternant and non-alternant hydrocarbons.

EFFECTS OF STRUCTURE ON REACTIVITY: Linear free energy relationships (LFER), the Hammett equation – substituent and reaction constants; the Taft treatment of polar and steric effects in aliphatic compounds

SECTION B

NUCLEOPHILIC SUBSTITUTION AT SATURATED CARBON: Mechanism and Stereochemistry of S_N1 and S_N2 , S_Ni reactions. The reactivity effects of substrate structure, solvent effects, competition between S_N1 and S_N2 mechanisms

SECTION C

ELECTROPHILIC AROMATIC SUBSTITUTION: The Arenium ion mechanism, orientation and reactivity in monosubstituted benzene rings, ortho/ para ratio. Ipso substitution

NUCLEOPHILIC AROMATIC SUBSTITUTION: The Aromatic S_N1 , S_N2 and benzyne mechanisms. Reactivity – effect of substrate structure, leaving group, and attacking nucleophile.

SECTION D

NEIGHBOURING GROUP PARTICIPATION: Evidences of N.G.P.; the phenonium ion, participation by π and σ bonds, Anchimeric assistance. Classical versus non-classical carbonium ions—the present status.

Books recommended

1. M.B. Smith & Jerry March, March's Advanced Organic Chemistry, 5th Edition (2001), John Wiley & Sons, New York.
2. Peter Sykes, A Guide book to Mechanism in Organic Chemistry, 6th Edition (1997), Orient Longman Ltd., New Delhi.
3. S. M. Mukherjee and S.P. Singh, Reaction Mechanism in Organic Chemistry, 1st Edition (1990), Macmillan India Ltd., New Delhi.
4. T.H. Lowry and K.S. Richardson, Mechanism and Theory in Organic Chemistry, 3rd Edition (1998), Addison – Wesley Longman Inc. (1st Edition)
5. P.S. Kalsi, Organic Reactions and their Mechanisms, 1st Edition (1996), New Age International Publication, New Delhi.
6. I. L. Finar, *Organic Chemistry*, Vol. II, 5th Edition (1975) Reprinted in 1996, ELBS and Longman Ltd, New Delhi
7. R.T. Morrison and R.N. Boyd, Prentice: Organic Chemistry, 6th Edition.

| | |
|--------------------------|---|
| Course Title/Code | Physical Chemistry-I (CHH-503-T) |
| Course Type | Core |

| | |
|--|--|
| Course Nature L-T-P-O Structure | Hard 4-0-0-0 |
| Objectives | To impart knowledge of electrochemistry and kinetics of chemical reactions. To impart knowledge of surface chemistry and catalysis To impart knowledge of advance thermodynamics |
| Outcome | Students will be able to understand concepts of electrochemistry and kinetics of chemical reactions Students will be able to understand the role of catalyst on its absorption behavior |
| Prerequisites | B.Sc. with Chemistry as one of the Subject |

| Syllabus | Sections | Weightage |
|----------|----------|-----------|
| | A | 25% |
| | B | 25% |
| | C | 25% |
| | D | 25% |
| | TOTAL | 100% |

SECTION-A

ELECTROCHEMISTRY: Metal/Electrolyte interface: OHP and IHP, potential profile across double layer region, potential difference across electrified interface; Structure of the double layer : Helmholtz-Perrin, Gouy-Chapman, and Stern models. Butler-Volmer equation under near equilibrium and non-equilibrium conditions, exchange current density, Tafel plot. Polarizable and non-polarizable interfaces. Derivation of the Debye-Huckel theory of activity coefficients (both point ion size and finite ion size models).

SECTION-B

CHEMICAL KINETICS : Composite Reactions - types of composite mechanisms, rate equations for composite mechanisms, simultaneous and consecutive reactions, steady state treatment, rate determining steps, microscopic reversibility and detailed balance, dynamic chain (H_2-Br_2) reaction, decomposition of ethane and acetaldehyde) and oscillatory reactions (Belousov-Zhabotinskii reaction), branching chain : H_2-O_2 reaction. Theory of unimolecular reactions, Lindemann mechanism, Hinshelwood treatment, RRKM model (qualitative treatment).

SECTION-C

SURFACE CHEMISTRY AND CATALYSIS: Interphase region, curved surfaces. Thermodynamics of surfaces : Gibbs adsorption isotherm, heat and entropy of adsorption. Surface film on liquids; Electro-kinetic phenomena. Catalytic activity at surfaces (volcano curve), Surface area determination (BET equation), transition state theory of surface reactions: rates of chemisorption and desorption, unimolecular and bimolecular surface reactions, comparison of homogeneous and heterogeneous reaction rates, surface heterogeneity, lateral interaction.

SECTION-D

THERMODYNAMICS: Partial molar properties and their significance. Fugacity : its concept and determination. Properties of ideal solutions; non-ideal systems-deviations (negative and positive) from ideal behaviour, excess functions for non-ideal solutions, calculations of partial molar quantities, determination of partial molar volume and partial molar enthalpy.

Books Recommended

1. O'.M. Bockris and A. K. N. Reddy, Modern Electrochemistry, Vol. 2 A & B, Second Edition (1998), Plenum Press, New York.
2. K. J. Laidler, Harper & Row, Chemical Kinetics, Third Edition (1987, New York.
3. P. W. Atkins, Physical Chemistry, Seventh Edition (2002), Oxford University Press, New York.
4. I.N. Levine, Physical Chemistry, 5th Edition (2002), Tata McGraw Hill Pub. Co. Ltd., New Delhi.
5. J. Raja Ram and J.C. Kuriacose, Kinetics and Mechanism of Chemical Transformations (1993), MacMillan Indian Ltd., New Delhi.

| | |
|--|--|
| Course Title/Code | ANALYTICAL CHEMISTRY (CHH504-T) |
| Course Type | Core |
| Course Nature L-T-P-O Structure | Hard 4-0-0-0 |
| Objectives | To impart knowledge on various analytical techniques To familiarize with the principle of analytical chemometrics |
| Outcome | Students will be able to Understand various analytical techniques Students will be able to understand factor analysis, resolution and pattern recognition |
| Prerequisites | B.Sc. with Chemistry as one of the Subject |

| Syllabus | Sections | Weightage |
|----------|----------|-----------|
| | A | 25% |
| | B | 25% |
| | C | 25% |
| | D | 25% |
| | TOTAL | 100% |

SECTION A

INTRODUCTION: Scope & objectives, Analytical chemistry and chemical analysis, Classification of analytical methods, Method selection, Sample processing, Steps in a quantitative analysis, Quantitative range (bipartite classification), Data organization, analytical validations, Limit of detection and limit of quantization, The tools of analytical chemistry and good lab practices.

SECTION B

TECHNIQUES IN ANALYTICAL CHEMISTRY-I

Polarography: Origin of polarography, Current-voltage relationship, Theory of polarographic waves (DC and sampled DC (tast) polarograms), Instrumentation, Ilkovic equation, Qualitative and quantitative applications.

SECTION C

TECHNIQUES IN ANALYTICAL CHEMISTRY-II

Spectroscopic Techniques: Theory, Instrumentation and applications of X-rays (emission, absorption, diffraction and fluorescence methods), Atomic absorption Spectroscopy, Atomic fluorescence spectrometry, Atomic emission spectrometry

Spectroscopy: UV-visible molecular absorption spectrometry (instrumentation and application), Molecular luminescence spectroscopy (fluorescence, phosphorescence, chemiluminescence).

SECTION D

TECHNIQUES IN ANALYTICAL CHEMISTRY-III

Separation Methods: Principle of chromatography, Classifications of chromatography, Techniques of planar and column chromatography, Gas chromatography, High-performance liquid chromatography

Thermal Analysis: Theory, methodology and applications of thermogravimetric analysis (TGA), Differential Thermal Analysis (DTA), and Differential scanning calorimetry (DSC). Principles, techniques and applications of thermometric titration methods.

Books Recommended

1. D.A. Skoog, *Principles of Instrumental Analysis*, 5th Edition (1998), Saunders College Publishing, Philadelphia, London.
2. G.W. Ewing, *Instrumental Methods of Chemical Analysis*, 5th Edition (1978), McGraw Hill Books Co., New York.
3. R.L. Pecsok, L. D. Shields, T. Cairns and L.C. Mc William, *Modern Methods of Chemical Analysis*, 2nd Edition (1976), John Wiley, New York.
4. J.H. Kennedy, *Analytical Chemistry: Principles*, 2nd Edition (1990), Saunders Holt, London.
5. R. L. Pecsok, L. D. Shields, T. Cairns and L.C. Mc William, *Modern Methods of Chemical Analysis*, 2nd Edition (1976), John Wiley, New York.
6. G. D. Christian, *Analytical Chemistry*, 5th Edition (1994), John Wiley & Sons, New York.
7. D. A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, *Analytical Chemistry - An Introduction*, 7th Edition (2000), Saunders College Publishing, Philadelphia, London.
8. D.C. Harris. *Quantitative Chemical Analysis*, 7th Edition.

| | |
|--|--|
| Course Title/Code | LABORATORY WORK-I (CHH505-P) |
| Course Type | Core |
| Course Nature L-T-P-O Structure | Hard 0-0-8-0 |
| Objectives | To Familiarize students with gravimetric and volumetric analysis of inorganic complex compounds To Familiarize students with identification of organic compounds having one or more functional groups |
| Outcome | The students will be able to gravimetric and volumetric analysis inorganic complex compounds The students will be able to understand qualitative analysis of mixture containing five rare cations |
| Prerequisites | B.Sc. with Chemistry as one of the Subject |

INORGANIC CHEMISTRY PRACTICAL (GRAVIMETRIC AND VOLUMETRIC ANALYSIS)

1. To estimate iron as Ferric oxide in a solution of ferrous sulphate or ferrous ammonium sulphate.
2. To estimate Aluminium or aluminium oxide in potash alum or ammonium aluminium sulphate.
3. To estimate the amount of ferric ion volumetrically and nickel gravimetrically.
4. To estimate amount of calcium volumetrically and barium gravimetrically.

Inorganic Synthesis

1. Sodium Ferrioxalate $\text{Na}_3[\text{Fe}(\text{C}_2\text{O}_4)_3] \cdot 9\text{H}_2\text{O}$
2. Nickel Dimethylglyoxime Complex $[\text{Ni}(\text{DMG})_2]$
3. Tetraamminecopper (II) sulphate, $[\text{Cu}(\text{NH}_3)_4]\text{SO}_4$

ORGANIC CHEMISTRY PRACTICAL

1. One step synthesis of organic compounds.
2. Identification of organic compounds in given mixtures.

PHYSICAL CHEMISTRY PRACTICAL

1. Saponification of ethyl acetate with sodium hydroxide by chemical method.

2. Comparison of acid strengths through acid catalyzed methyl acetate hydrolysis.
3. Distribution coefficient of I_2 , WO between two immiscible solvents.
4. Conductometric titration of a weak acid with strong base.
5. Potentiometric titrations and determination of dissociation constant of different mixtures and salts.

| | |
|--------------------------|---|
| Course Title/Code | Workshop (CHW506) |
| Course Type | Core |
| Course Nature | Hard |
| L-T-P-O Structure | 0-0-3-0 |
| Objectives | To Familiarize students with inorganic synthesis To expose the students with the synthesis of organic compounds and intermediates. To familiarize students with conductometric and potentiometric titrations. |

INORGANIC ANALYSIS:

1. Qualitative analysis of mixtures of salts including rare element salts (soluble and insoluble) containing eight radicals including interfering
2. Qualitative analysis of mixtures of metal ions by complexometric titrations (mixture of two metals) with the use of masking and demasking agents.
3. TLC : preparation and analysis
4. Preparation of compounds and intermediates involving up to two steps.
5. Determination of solubility product of sparingly soluble salt conductometrically.
6. Conductometric titration of a mixture of weak and strong acids.

| | |
|---------------------------|--|
| Course Title/ Code | Research Methodology/PHS 501 |
| Course Type | Allied Core |
| Course Nature | Soft |
| L-T-P Structure | (1-0-2) |
| Objectives | Student shall be able to apply the fundamentals of research methodology to a problem and make an informed decision. |
| Outcome | Student shall be able to CO1: write hypothesis; generate and choose alternatives; and test hypothesis. CO2: select a sample ; generate data and present it CO3: Calculate averages and dispersion CO4: Calculate correlation and regression. |

SECTION A

Basic Concepts of Research; Formulation & steps of Research : Decision-making: identifying the problem & Steps of decision-making process. Research : Its objectives and types. Formulation of Research Problem; its components and sources. Steps of research & Research ethics. Performance monitoring in research

Research Design: Requirements of Research Design; Types of Research Design; Factors Affecting Research Design; Hypothesis Formulation; Hypothesis Testing

SECTION B

Sampling Methods and Techniques: Sampling design; Scope of sampling method; Laws of sampling; Determination of sample size; Techniques of sampling.

Properties of Data Collection and Measurement : Basic Characteristics of data; Types of data and Scaling measurement. Methods of primary data collection; Editing Raw Data; Coding of Data; Tabulation of Data; Constructing Charts.

Presentation of Results : Report writing: Purpose of a Report; Essentials of a Good Report; Format of a Report; Types of Report Presentation.

SECTION C

Measures of Central Tendency: Types of Averages: The Arithmetic Mean; The Weighted Arithmetic Mean; The Median; The Mode; The Geometric Mean; The Harmonic Mean

Measures of Dispersion: Definition; Methods of Measuring Dispersion; The Range; The Inter-quartile Range; The Mean/Average Deviation ; The Standard Deviation; The Coefficient of Variation; The Gini Coefficient and the Lorenz Curve

Matrix Algebra : Matrix Multiplication; Matrix Addition; Matrix Substitution; Transpose of the Product of Two Matrices; Inverse of a Square Matrix; Matrix Notation in Case of Regression Analysis

SECTION D

Multivariate Analysis; Correlation & Regression Analysis: Factor Analysis; Discriminant Analysis; Cluster Analysis; Dimensional Analysis; Meta Analysis; Conjoint Analysis. Introduction to Correlation Analysis; Rank Correlation; Linear Regression Analysis; Multiple Regression Analysis

Laboratory Work:

1. Identifying the hypothesis; alternatives and situations in given abstracts/reports.

2. Writing a research proposal as per research design fundamentals.
3. Coding, tabulating and drawing charts for a given data.
4. Calculating & plotting averages for the given data
5. Measuring dispersion for the given data.
6. Calculating correlation for the given data.
7. Calculating regression for a given data.

Mini Project: Identify a problem in given environment and apply the concepts of research methodology to conduct research and present the results.

Text Books:

1. Research Methodology by Dr. Prashant Sarangi. Taxmann Publications Pvt Ltd

SEMSETER II

| COURSE CODES | COURSE NAME | COURSE TYPE | COURSE NATURE | PERIODS | | | | NO. OF CONTACT HOURS PER WEEK | CREDITS |
|--------------|------------------------|--|---------------------------------|---------|---|---|---|-------------------------------|---------|
| | | Core(Departmental/Allied)/ Elective (Departmental/ Open) / University Compulsory | Hard/Soft/ Workshop/ NTCC | | | | | | |
| CHH508-T | INORGANIC CHEMISTRY-II | CORE(Departmental) | HARD | 4 | 0 | 0 | 0 | 4 | 4 |
| CHH509-T | ORGANIC CHEMISTRY-II | CORE(Departmental) | HARD | 4 | 0 | 0 | 0 | 4 | 4 |
| CHH510-T | PHYSICAL CHEMISTRY-II | CORE(Departmental) | HARD | 4 | 0 | 0 | 0 | 4 | 4 |
| CHH511-T | SPECTROSCOPY | CORE(Departmental) | HARD | 4 | 0 | 0 | 0 | 4 | 4 |
| CHH512-P | LABORATORY WORK-II | CORE(Departmental) | HARD | 0 | 0 | 8 | 0 | 8 | 4 |
| CHW513 | WORKSHOP | CORE(Departmental) | WORKSHOP | 0 | 0 | 3 | 0 | 3 | 2 |
| MES 515 | RESEARCH PAPER WRITING | CORE (Allied) | SOFT | 1 | 0 | 2 | 0 | 3 | 2 |
| CHW514 | SUMMER TRAINING | | | | | | | | 3 |

**DETAILED SYLLABUS
CHP01 –SECOND SEMESTER**

| | |
|--|--|
| Course Title/Code | Inorganic Chemistry-II (CHH508-T) |
| Course Type | Core |
| Course Nature L-T-P-O Structure | Hard 4-0-0-0 |
| Objectives | To familiarize with kinetics of substitution reactions To impart knowledge on electron transfer reactions |
| Outcome | The students will be able to understand Kinetics and Mechanism of Substitution Reactions The students will be able to understand electron transfer reaction |
| Prerequisites | Inorganic Chemistry-I |

| Syllabus | Sections | Weightage |
|----------|----------|-----------|
| | A | 25% |
| | B | 25% |
| | C | 25% |
| | D | 25% |
| | TOTAL | 100% |

SECTION-A

KINETICS AND MECHANISM OF SUBSTITUTION REACTIONS: Nature of substitution reactions; prediction of reactivity of octahedral, tetrahedral, trigonal bipyramidal and square-planar complexes in terms of VBT and CFT; rates of reactions; acid hydrolysis, base hydrolysis and anation reactions.

SECTION-B

ELECTRON TRANSFER REACTIONS: Mechanism and rate laws; various types of electron transfer reactions, Marcus-Hush theory, correlation between thermal and optical electron transfer reactions; identification of inter valence transfer bands in solution.

SECTION-C

METAL CARBONYLS: Preparation and structure; vibrational spectra of metal carbonyls, reactions of metal carbonyls.

SECTION-D

OPTICAL ROTATORY DISPERSION AND CIRCULAR DICHROISM: Linearly and circularly polarized lights; optical rotatory power and circular birefringence, ellipticity and circular dichroism; ORD and Cotton effect, Faraday and Kerr effects; Assignment of electronic transitions; applications of ORD and CD for the determination of (i) absolute configuration of complexes and (ii) isomerism due to non-planarity of chelate rings.

Books Recommended

- 1 F. Basalo and R. G. Pearson, *Mechanism of Inorganic Reactions*, 2 nd Edn (1967), Wiley Eastern Ltd., New Delhi.
- 2 D. F. Shriver and P. W. Atkins, *Inorganic Chemistry*, 3 rd Edn. (1999), ELBS, London.
- 3 F. A. Cotton and G. Wilkinson, *Advanced Inorganic Chemistry*, 6 th Edn. (1999), John Wiley & Sons, New York.
4. D.N. Sathyanarayana, *Electronic Absorption Spectroscopy and Related Techniques* (2001), Universities Press (India) Ltd., Hyderabad.
5. K.F. Purcell, J.C. Kotz, *Inorganic chemistry*, Saunders 1977.

| | |
|--------------------------|--|
| Course Title/Code | Organic Chemistry-II (CHH509-T) |
| Course Type | Core |
| Course Nature | Hard |
| L-T-P-O Structure | 4-0-0-0 |
| Objectives | To familiarize with electrophilic, free-radical and nucleophilic addition reactions To impart knowledge on esterification and Elimination reactions |
| Outcome | Students will be able to understand the mechanism of electrophilic, free-radical and nucleophilic addition reactions Students will be able to explain the mechanism of esterification and Elimination reactions |
| Prerequisites | Organic Chemistry-I |

| Syllabus | Sections | Weightage |
|----------|----------|-----------|
| | A | 25% |
| | B | 25% |
| | C | 25% |
| | D | 25% |
| | TOTAL | 100% |

SECTION A

ADDITION TO CARBON–CARBON MULTIPLE BONDS: Electrophilic, free-radical and nucleophilic addition: Mechanistic and Stereo chemical aspects. Orientation and reactivity, Hydroboration and Michael reaction

SECTION B

ESTERIFICATION AND HYDROLYSIS OF ESTERS: Evidence for tetrahedral intermediate in BAc2 and AAc2 mechanisms, steric and electronic effects. The AAc1 and other pathways involving alkyl to oxygen bond cleavage

SECTION C

ELIMINATION REACTIONS: The E1, E2 and E1Cb (Elimination Unimolecular conjugate Base) mechanisms, Orientation of the double bond. Hofmann versus Saytzeff elimination, Pyrolytic syn-elimination, Competition between substitution and elimination reactions

KINETIC ISOTOPE EFFECTS: Its origin and importance in determining reaction mechanism, Solvent isotope effects.

SECTION D

CONSERVATION OF ORBITAL SYMMETRY IN PERICYCLIC REACTIONS: Woodward-Hoffmann rules; cycloaddition [2+2] and [4+2], and electrocyclic reactions, Prototropic and Sigmatropic rearrangements, Ene reactions and Chelotropic reactions; 1,3-Dipolar cycloaddition

Books recommended

1. M.B. Smith & Jerry March, March's Advanced Organic Chemistry, 5th Edition (2001), John Wiley & Sons, New York.
2. Peter Sykes, A Guide Book to Mechanism in Organic Chemistry, 6th Edition (1997), Orient Longman Ltd., New Delhi.
3. S. M. Mukherjee and S.P. Singh, Reaction Mechanism in Organic Chemistry, 1st Edition 1990), Macmillan India Ltd., New Delhi.
4. T.H. Lowry and K.S. Richardson, Mechanism and Theory in Organic Chemistry, 3rd Edition (1998), Addison – Wesley Longman Inc. (1st Edition).
5. P. S. Kalsi, Organic Reactions and Their Mechanisms, 1st Edition (1996), New Age International Pub., New Delhi.
6. S.M. Mukherjee and S.P. Singh, Pericyclic Reactions, MacMillan India, New Delhi.
7. I. Fleming, Pericyclic Reactions, Oxford University Press, Oxford (1999).

| | |
|--|--|
| Course Title/Code | Physical Chemistry-II (CHH510-T) |
| Course Type | Core |
| Course Nature L-T-P-O Structure | Hard 4-0-0-0 |
| Objectives | To familiarize with concept of corrosion cyclic voltammetry To impart knowledge of Statistical Thermodynamics |
| Outcome | Students will be able to understand corrosion cause and type Students will be able to understand Statistical Thermodynamics in relation to the Concepts of distribution and thermodynamic probability |
| Prerequisites | Physical Chemistry-I |

| Syllabus | Sections | Weightage |
|----------|----------|-----------|
| | A | 25% |
| | B | 25% |
| | C | 25% |
| | D | 25% |
| | TOTAL | 100% |

SECTION-A

ELECTROCHEMISTRY: CORROSION: Scope and economics of corrosion, causes and types of corrosion, electrochemical theories of corrosion, kinetics of corrosion (corrosion current and corrosion potential). Corrosion measurements (weight loss, OCP measurement, and polarization methods), units of corrosion rate passivity and its breakdown, corrosion, prevention (electrochemical, inhibitor, and coating methods).

CYCLIC VOLTAMMETRY: Cell design, instrumentation, current-potential relation for linear sweep voltammetry (LSV), cyclic voltammetry.

SECTION-B

STATISTICAL THERMODYNAMICS: Concepts of distribution, thermodynamic probability and most probable distribution. Ensemble averaging, postulates of ensemble averaging, Boltzmann distribution of particles. Types of statistics: Maxwell- Boltzmann, Bose-Einstein and Fermi-Dirac statistics. Idea of microstates and macrostates. Thermodynamic probability (W) and derivation of distribution laws for three types of statistics.

PARTITION FUNCTION: translational, rotational, vibrational partition functions, thermodynamic properties of ideal gases in terms of partition function.

SECTION-C

MICELLES: Surface active agents and their classification, micellization, hydrophobic interaction, critical micellar concentration (cmc), factors affecting cmc of surfactants, counter ion binding to micelles, thermodynamics of micellization-phase separation and mass action models, solubilization, micro emulsions, reverse micelles.

MACROMOLECULES: Polymers-definition, types of polymers, liquid crystal polymers. Molecular mass-number and mass average molecular mass, determination of molecular mass (osmometry, viscosity, diffusion, light scattering, and sedimentation methods).

SECTION-D

NUCLEAR CHEMISTRY: Nuclear stability and binding energy. Mass and binding energy systematics. Nuclear isomerism and internal conversion, Nuclear fission and nuclear fusion- fission cross section, chain fission, fission product and fission yield, mass and charge distribution in fission, Nuclear fusion and stellar energy.

Books Recommended-

1. J.O'M. Bockris and A. K. N. Reddy, *Modern Electrochemistry*, Vol. 2, Second Edition, (1998) Plenum Press, New York.
2. P. W. Atkins, *Physical Chemistry*, 7th Edition, (2002) Oxford University Press, New York.
3. I. N. Levine, *Physical Chemistry*, 5th Edition (2002), Tata McGraw Hill Pub. Co. Ltd., New Delhi.
4. Andrew Maczek, *Statistical Thermodynamics*, (1998) Oxford University Press Inc., New York.
5. Y. Moroi, *Micelles : Theoretical and Applied Aspects*, (1992) Plenum Press, New York.
6. F.W. Billmeyer, Jr., *Text Book of Polymer Science*, 3rd Edition (1984), Wiley-Interscience, New York.
7. B. G. Harvey, *Introduction to Nuclear Physics and Chemistry*, (1969) Prentice Hall, Inc.
8. H.J. Arnikar, *Essentials of Nuclear Chemistry*, 4th Edition (1995), Wiley-Eastern Ltd., New Delhi.
9. Friedlander, G., and Kennedy, J. W., *Nuclear and Radio-chemistry*, John Wiley & Sons, Inc., New York, 1955.

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|--|--|
| Course Title/Code | SPECTROSCOPY (CHH511-T) |
| Course Type | Core |
| Course Nature L-T-P-O Structure | Hard 4-0-0-0 |
| Objectives | To familiarize with PMR and CMR To impart knowledge on mass spectroscopy for studying the fragmentation pattern |
| Outcome | Students will be able to understand principle of PMR, CMR and ESR spectroscopy Students will be able to understand Photoelectron Spectroscopy Students will be able to analysis fragmentation pattern of the compound by mass spectrometry |
| Prerequisites | B.Sc. with Chemistry as one of the Subject |

| Syllabus | Sections | Weightage |
|----------|----------|-----------|
| | A | 25% |
| | B | 25% |
| | C | 25% |
| | D | 25% |
| | TOTAL | 100% |

SECTION A

SPECTROSCOPY-I

PMR: Natural abundance of ^{13}C , ^{19}F and ^{31}P nuclei, the spinning nucleus, effect of external magnetic field, precessional motion and frequency Energy transitions Chemical shift and its measurements, factors influencing chemical shift, anisotropic effect, integral of protons spin spin coupling splitting theory magnitude of coupling constant simple, virtual and complex spin coupling , Chemical and magnetic equivalence proton exchange, factors affecting the coupling- First and non first order spectra, simplification of complex spectra (solvent effect, double resonance and field effect)

SECTION B

CMR: Resolution and multiplicity of ^{13}C NMR, ^1H -decoupling noise decoupling, broad band decoupling, Deuterium, fluorine and phosphorus coupling, NOE signal enhancement off-resonance, proton decoupling, structural application of CMR DEPT and INEPT experiments, Introduction to 2D NMR .

SECTION C

ESR: Derivative curves hyperfine splitting, g value, ESR spectra of simple molecules

Mass: Theory, instrumentation and modification Unit mass and molecular ions Important terms singly, double/multiple charged ion metastable peak base peak isotopic mass peak, relative intensity etc.

SECTION D

Photoelectron Spectroscopy: Principle and Instrumentation, Types of Photoelectron Spectroscopy – UPS & XPS Binding Energies, Koopman's Theorem, Chemical Shifts. Photoelectron Spectra of Simple Molecules: N_2 , O_2 , F_2 , , CO , HF , NH_3 and H_2O - Vibrational Structure of PES Bands, Potential energy curves, Interpretation of Vibrational spectral data for ionized (M^+) species, Prediction of Nature of Molecular Orbitals. ESCA in qualitative analysis, Principles of Auger electron spectroscopy.

Books Recommended-

1. R.M. Silverstein and F.X. Webster, Spectroscopic identification of organic compounds
2. William Kemp, Organic spectroscopy 3rd edition.
3. M. Rose and R.A. W. Johnstone, Mass Spectrometry for Chemists and biochemists
4. D.H. Williams and I. Fleming, Spectroscopic methods in organic chemistry
5. Donald L.Pavia and G.M.Lampman, Introduction to Chemistry

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|--|---|
| Course Title/Code | LABORATORY WORK-II (CHH512-P) |
| Course Type | Core |
| Course Nature L-T-P-O Structure | Hard 0-0-8-0 |
| Objectives | To familiarize students with Quantitative separation and determination of metal ions |
| Outcome | Students will be able to understand Quantitative separation and determination of metal ions |
| Prerequisites | Nil |

INORGANIC CHEMISTRY PRACTICALS

1. Quantitative separation and determination of the following pairs of metal ions using gravimetric and volumetric methods. For example: Ag^+ (gravimetrically) and Cu^{2+} (volumetrically), Cu^{2+} (gravimetrically) and Zn^{2+} (volumetrically), Fe^{3+} (gravimetrically) and Ca^{2+} (volumetrically), Mg^{2+} (gravimetrically) and Ca^{2+} (volumetrically) etc.

ORGANIC CHEMISTRY PRACTICALS

1. Preparation of compounds involving not more than two steps.
2. Identification of organic compounds in given mixture.

PHYSICAL CHEMISTRY PRACTICALS

1. Rate constant of acid catalyzed hydrolysis of sucrose by polarimetric method.
2. Rate constant of acid catalyzed hydrolysis of sucrose by chemical method.
3. Rate constant of FeCl_3 -catalyzed H_2O decomposition by gasometric method.
4. Degree of hydrolysis of urea hydrochloride by kinetics method.

| | |
|--------------------------|--|
| Course Title/Code | Workshop (CHW513) |
| Course Type | Core |
| Course Nature | Hard |
| L-T-P-O Structure | 0-0-3-0 |
| Objectives | To familiarize students with Preparation of compounds involving not more than two steps To expose the students with polarimetric method to determine rate constant. |

1. Separation of a mixture of cations/anions by paper chromatographic technique using aqueous/non-aqueous media. For example: Pb²⁺ and Ag⁺ (aqueous & non-aqueous media), Co²⁺ and Cu²⁺ (non-aqueous medium), Cl⁻ and I⁻ (aqueous-acetone medium), Br⁻ and I⁻ (aqueous-acetone medium) etc.
2. Systematic identification of mixtures containing two organic compounds
3. Equilibrium constant of $KI + I_2 \rightleftharpoons KI_3$ by distribution method.

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|---------------------------|---|
| Course Title/ Code | RESEARCH PAPER WRITING / SEMINAR (RPW / S) |
| Course Code | MES 515 |
| Course Type | DOMAIN CORE |
| Course Nature | SOFT COURSE |
| L-T-P-O Structure | 1-0-2-0 |
| Objectives | To acquaint the researcher with the tools of research by exposing them to the mechanics of writing a research report/ research paper/ thesis/ dissertation. |

| | |
|--------------------------|---|
| Learning Outcomes | <p>Upon completion of this course, the students should be able to:</p> <ul style="list-style-type: none"> • Know what formats, designs, structure and styles to use to best get their ideas, concepts and messages across in a way that is clear and unambiguous. • Be capable of recognising and correcting many common errors that currently occur within written communication in the technical field. • Produce different types of Technical Reports for various purposes • Use clear and powerful language to target and persuade readers for positive results • Produce documents of a high professional standard. |
|--------------------------|---|

| Syllabus | Sections | Weightage |
|----------|--------------|-------------|
| | A | 25% |
| | B | 25% |
| | C | 25% |
| | D | 25% |
| | TOTAL | 100% |

SECTION A

Research Paper:- Definition, Quality of a good Research Paper, Report Paper and Thesis Paper; Details of a Research Paper – Steps and Schedule.

Choosing a Topic:- Brainstorming, Consulting Experts, Considering Parameters, Narrowing the Research Topic.

Thesis:- Definition and function, Outline, Thesis Statement

SECTION B

Doing Research:- Finding Information, Sources of Information; Online Resources, Search Engines, Databases, Newsgroups, Internet Sites; Library – Books, Research Papers, Periodicals, Magazines and Journals,, Interviews, Surveys, Government Documents, Pamphlets, Special Collections; Evaluating Sources

Taking Notes:- Reading, Notes Taking Methods, Guidelines and Summarizing

SECTION C

Rough Draft :- Transforming Notes into Rough Draft Creating Outlines, Types of Outlines; Basics of Research Paper Style ; Words, Sentences, Punctuation ; Writing Introduction; Using Notes, Quotations, Graphics etc.

Revising Rough Drafts:- Principles, Revising Opening Paragraph, Sentences, Words and Rules for Writers, Plagiarism and how to avoid it, Plagiarism Detection Programs.

SECTION D

Documentation :- MLA System of Documentation ; Parenthetical Documentation, Format for Work Cited, Using Footnotes and Endnotes to Document Sources and add Observations and Comments – Guidelines and Format ; APA System of Documentation, Traditional System of Documentation (CMS).

Presentation of Research Paper:- Title Page, Table of Contents, Forward and Preface, Abstract, Presentation Footnote. Finished Form of Paper – Revising, Editing, Proofreading, Peer Review Checklist, Submitting Electronically. Model Research Papers.

Reference Books:

- 1) Gibaldi, Joseph. *MLA Handbook for Writers of Research Papers*. 7th ed. New Delhi: East-West Press, 2009
- 2) Kothari, C.R. *Research Methodology: Methods and Techniques*. New Delhi: New Age International Ltd, 1985.
- 3) Rahim, F. Abdul. *Thesis Writing: A Manual for Researchers*. New Delhi: New Age International Pvt Ltd, 1996.
- 4) Laurie Rozakis, *Schaum's Quick Guide to Writing Great Research Papers*, M/cGraw- Hill 2007.
- 5) Anthony C. Winkler / Jo Ray McCuen –Metherel, *Writing the Research Paper*. Wadsworth Cengage Learning. 2008

LABORATORY

Report writing consisting of about 1,000 words, on any subject of the student's choice, in the field of research in Mechanical Engineering.

Prepare atleast two Research Papers in IEEE & Science Direct Format. Your **research paper** must be 3 pages **minimum** plus reference page, typed (approx. 250 words per page) on a technical topic of the student's choice dealing the field of research in Mechanical.

Seminar presentation, on Report Writing and Research Papers.

SEMESTER III

| COURSE CODES | COURSE NAME | COURSE TYPE | COURSE NATURE | PERIODS | | | | NO. OF CONTACT HOURS PER WEEK | CREDITS |
|----------------------|---|-------------------------|---------------|---------|---|---|---|-------------------------------|---------|
| | | | | L | T | P | O | | |
| CHH615-T | CONFORMATIONAL ANALYSIS, ASYMMETRIC SYNTHESIS & BIOMOLECULES | CORE(Departmental) | HARD | 4 | 0 | 0 | 0 | 4 | 4 |
| CHH616-T | MODERN ORGANIC SYNTHETIC TECHNIQUES & STEREOCHEMISTRY | CORE(Departmental) | HARD | 4 | 0 | 0 | 0 | 4 | 4 |
| CHH617-T CHH618-T | ELECTIVE-I (A) BIO-INORGANIC CHEMISTRY AND ORGANOMETALLIC CHEMISTRY & (B) DRUG DESIGN | ELECTIVE (Departmental) | HARD | 4 | 0 | 0 | 0 | 4 | 4 |
| CHH619-T | PHOTOCHEMISTRY & PERICYCLIC REACTIONS | CORE(Departmental) | HARD | 4 | 0 | 0 | 0 | 4 | 4 |

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|----------|---------------------|--------------------|------|---|---|---|---|---|---|
| CHH620-P | LABORATORY WORK-III | CORE(Departmental) | HARD | 0 | 0 | 6 | 0 | 6 | 3 |
| CHH621-P | LABORATORY WORK-IV | CORE(Departmental) | HARD | 0 | 0 | 6 | 0 | 6 | 3 |
| CHN622 | SEMINAR | CORE(Departmental) | | 0 | 0 | 0 | 2 | 2 | 2 |

**DETAILED SYLLABUS
CHP01 –THIRD SEMESTER**

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|--------------------------|---|
| Course Title/Code | CONFORMATIONAL ANALYSIS AND ASYMMETRIC SYNTHESIS & BIOMOLECULES (CHH615-T) |
| Course Type | Core |
| Course Nature | Hard |
| L-T-P-O Structure | 4-0-0-0 |
| Objectives | To make the students familiarize about the conformations of basic organic compounds To introduce to the students the basic terminology, nomenclature and conditions involved in asymmetric synthesis To familiarize the students with the enzyme catalyzed reactions To make the students understand the structures of various nucleic acids |
| Outcome | The student will be able to learn about the conformational analysis of various organic compounds The student will be able to understand the principles of asymmetric syntheses The student will be able to write the mechanism of enzyme catalyzed reactions and synthesis of nucleic acids |
| Prerequisites | Organic Chemistry-I & II |

| Syllabus | Sections | Weightage |
|----------|----------|-----------|
| | A | 25% |
| | B | 25% |
| | C | 25% |
| | D | 25% |
| | TOTAL | 100% |

SECTION A

CONFORMATIONAL ANALYSIS (CYCLIC SYSTEMS): Study of conformations of cyclohexane, mono, di and polysubstituted cyclohexanes, cyclohexene, cyclohexanone (2-alkyl and 3-alkyl ketone effect), 2-halocyclohexanones, cyclopentane, cyclobutane, cycloheptane and cyclooctane, Stereochemistry of bicycle [3,3,0]octanes, hydrindanes, decalins and perhydroanthracenes.. Conformational effects on the stability and reactivity of diastereomers in cyclic molecules - steric and stereo electronic factors – examples, Factors governing the reactivity of axial and equatorial substituents in cyclohexanes, Stereochemistry of addition to the carbonyl group of a rigid cyclohexanone ring.

SECTION B

PRINCIPLES OF ASYMMETRIC SYNTHESIS: Introduction and terminology: Topicity in molecules Homotopic, stereoheterotopic (enantiotopic and diastereotopic) groups and faces- symmetry, substitution and addition criteria. Prochirality nomenclature: Pro-R, Pro-S, Re and Si. Stereoselective reactions: Substrate stereoselectivity, product stereoselectivity, enantioselectivity and diastereoselectivity. Conditions for stereoselectivity: Symmetry and transition state criteria, kinetic and thermodynamic control. Methods for inducing enantio and diastereoselectivity. Analytical methods: % Enantiomeric excess, enantiomeric ratio, optical purity, % diastereomeric excess and diastereomeric ratio.

SECTION C

METHODOLOGIES IN ASYMMETRIC SYNTHESIS: Strategies in Asymmetric Synthesis: 1. Chiral substrate controlled, 2. Chiral auxiliary controlled, 3. Chiral reagent controlled and 4. Chiral catalyst controlled.

1. Chiral Substrate controlled asymmetric synthesis: Nucleophilic additions to chiral carbonyl compounds. 1, 2-asymmetric induction, Cram's rule and Felkin-Anh model.

2. Chiral auxiliary controlled asymmetric synthesis: α -Alkylation of chiral enolates, azaenolates, imines and hydrazones. 1, 4 Asymmetric induction and Prelog's rule. Use of chiral auxiliaries in Diels-Alder reaction.

3. Asymmetric aldol reaction: Diastereoselective aldol reaction (chiral enolate & achiral aldehydes and achiral enolate & chiral aldehydes) its explanation by Zimmerman-Traxel model.

SECTION D

1. ENZYMES: Definition, Classification based on mode of action, Mechanism of enzyme catalysis, Lock and Key model and Induced-Fit model, Enantiomer, discrimination by Three-point Contact model. Factors affecting enzyme catalysis. Enzyme inhibition- reversible and irreversible inhibition, Enzymes in organic synthesis. Immobilised enzymes.

2. NUCLEIC ACIDS: Primary, secondary and tertiary structure of DNA. Types of mRNA, tRNA and rRNA, Replication, transcription and translation, Genetic code, Protein biosynthesis. Chemical Synthesis of nucleosides and nucleotides.

Books Recommended

1. D. Nasipuri, Stereochemistry of Organic Compounds-Principles & Applications, New Age International.
2. P.S. Kalsi, Stereochemistry of Organic Compounds- Conformation and Mechanism: New Age International.
3. Ernest L Eliel & Samuel H. Wilen, Stereochemistry of Carbon compounds.
4. R S Ward, Stereo selectivity in organic synthesis
5. Howard, S. I.; Morrison, J. D. Asymmetric Synthesis; Academic: New York. 1983; Vol. 2.
6. Nogradi. M. Stereoselective Synthesis.

| | |
|--------------------------|--|
| Course Title/Code | MODERN ORGANIC SYNTHETIC TECHNIQUES & STEREOCHEMISTRY (CHH616-T) |
| Course Type | Core |
| Course Nature | Elective |
| L-T-P-O Structure | 4-0-0-0 |
| Objectives | To familiarize the student with the various synthetic reagents for using group protection and oxidation reactions. To make the student understand the mechanism of various synthetic routes. To make the student understand the new techniques and concepts in organic synthesis Student will be familiarized with stereochemistry principles. |
| Outcome | The student will be able to write the mechanism of organic reactions. The student will be able to predict the structure of organic compounds by stereochemistry. |
| Prerequisites | Organic and Inorganic Chemistry-I & II |

| Syllabus | Sections | Weightage |
|----------|----------|-----------|
| | A | 25% |
| | B | 25% |
| | C | 25% |
| | D | 25% |
| | TOTAL | 100% |

SECTION A

ORGANOSILICONE COMPOUNDS: Preparation and applications in organic synthesis; Application of Pd (I) and Pd (II) complexes in organic synthesis-stille, Suzuki, Sonogashira coupling Hack Reaction

SECTION B

PREPARATION AND APPLICATION OF LITHIUM ORGANOCUPARATES; REDUCTION Stereochemistry stereoselection and mechanism of catalytic hydrogenation and metal ammonia reduction.

HYBRID TRANSFER REAGENTS: Sodium borohydride, sodium cynoborohydride, lithium aluminum hydride and alkoxy substituted LAH reducing agents, DIBL, Application of hydroboration

SECTION-C

STEREOCHEMISTRY-I Symmetry elements, D-L, R-S, E-Z and threo-erythro nomenclature, interconversion of Fischer, Newman, Sawhorse and flying wedge formulae, conformational analysis, enantiomerism and diastereomerism of simple, cyclic (chair and boat configuration) and acyclic systems. Axial and planar chirality, optical isomerism in allenes, biphenyls (atropoisomerism), spiranes, hemispiranes. elementary ideas about stereochemistry of tertiary amines, quaternary salts, sulphur and phosphorous compounds.

SECTION-D

STEREOCHEMISTRY-II

Topicity of ligands and faces, their nomenclature and prostereoisomerism, stereogenicity, chirogenicity, pseudoasymmetry and prochiral centre. stereospecific and stereoselective reaction. Elementary idea of principle categories of asymmetric synthesis, Cram's rule and its modification, Prelog rule and Horeaus rule. Stereochemistry of sugars- C1 and 1C conformations of hexoses, c 2'-endo and c3'-endo conformation of pentoses, homomorphous sugars, abnormal mutarotation and Δ -2 instability factor.

Books Recommended

1. Jerry March Advanced Organic Chemistry Reactions, Mechanism and Structure, , John Wiley.
2. F. A. Carey and R. J. Sundberg, Advanced Organic Chemistry.
3. Peter Sykes, Longman A Guide Book to Mechanism in Organic Chemistry.
4. R. T. Morrison and R. N. Boyd, Organic Chemistry, Prentice -Hall.
5. H. O. House, Benjamin. Modern Organic Reactions
6. R. O. C. Norman and J. M. Coxon, Principles of Organic Synthesis.
7. S. M. Mukherji and S. P.Singh. Reaction Mechanism in Organic Chemistry, Macmillan.
8. D. Nasipuri, Stereochemistry of Organic Compounds-Principles & Applications, New Age International.
9. P.S. Kalsi, Stereochemistry of Organic Compounds- Conformation and Mechanism: New Age International.

| | |
|--------------------------|--|
| Course Title/Code | ORGANOMETALIC CHEMISTRY OF TRANSITION METALS AND BIO INORGANIC CHEMISTRY (CHH617-T) |
| Course Type | Core |
| Course Nature | Elective |
| L-T-P-O Structure | 4-0-0-0 |

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| Objectives | Student will understand the synthesis of π -Complexes of unsaturated Molecules and metal carbonyls. Student will understand the synthesis of Transition Metal Compounds in Homogeneous Catalysis System Student will be exposed to role of metal ions in various biological systems and understand the role of various bio-inorganic molecules in therapeutic use. |
| Outcome | The student will be able to write the synthesis of π -Complexes of Unsaturated Molecules The student will be able to understand the use of Transition Metal Compounds in Homogeneous Catalysis and biological systems |
| Prerequisites | Organic Chemistry and Inorganic chemistry-I & II |

| Syllabus | Sections | Weightage |
|----------|----------|-----------|
| | A | 25% |
| | B | 25% |
| | C | 25% |
| | D | 25% |
| | TOTAL | 100% |

SECTION A

METAL CARBONYLS: Semibridging carbonyl group; metal nitrosyl carbonyls; tertiary phosphines and arsines as ligands; carbenes and carbynes.

π -COMPLEXES OF UNSATURATED MOLECULES: Preparation, bonding and structures of alkene, alkyne, allyl, dienyl and trienyl complexes; reactions with special reference to organic synthesis.

SECTION B

COMPOUNDS OF TRANSITION METAL-CARBON MULTIPLE BONDS Alkylidenes, alkylidynes, low valent carbenes and carbynes- synthesis, nature of bond, structural characteristics, nucleophilic and electrophilic reactions on the ligands, role in organic synthesis Transition Metal Compounds with Bonds to Hydrogen

SECTION D

TRANSITION METAL π -COMPLEXES

Transition metal π -complexes with unsaturated organic molecules, alkenes, alkynes, allyl, diene, dienyl, arene and trienyl complexes, preparations, properties, nature of bonding and structural features. Important reactions relating to nucleophilic and electrophilic attack on ligands and to organic synthesis.

SECTION-C

CATALYSIS: Transition metal ion catalysis for organic transformations and their application in hydrogenation (using symmetric and chiral catalysts), isomerization, olefin oxidation, carbonylation and polymerization reactions. Role of metal ions in biological systems.

SECTION-D

BIO-INORGANIC PROCESSES: Toxic metal ions and their detoxification, chelation therapy/chelating agents in medicine. Recent advances in cancer chemotherapy using chelates. Biological nitrogen fixation. Natural and synthetic oxygen carriers. Na-K, ATPase or sodium pump. Futuristic aspects of organo transition metal complexes as catalysts and in bio-inorganic chemistry.

Books Recommended

1. F. A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, 6th Edn., (1999), John-Wiley & Sons, New York.
2. James E. Huheey, Inorganic Chemistry, 4thEdn., (1993), Addison Wesley Pub. Co., New York
3. R.H.Crabtree, The Organometallic Chemistry of the Transition Metals, 1st Edn.(1988), John-Wiley & Sons, New York.
4. J. P. Collman, L. S. Hegedus, J.R. Norton and Richard G. Finke, Principles and Applications of Organotransition Metal Chemistry, 1st Edn.(1987), University Science Books, Mill Valley, California.
5. Katakis, D. and Gordon, G. mechanism of Inorganic Reactions John Wiley & Sons: N. Y (1987)
6. Hughes, M.N. The Inorganic Chemistry of Biological Processes, 2nd Edition, Wiley (1981)
7. Masters, C. Homogeneous transition Metal Catalysis Chapman and Hall (1981)

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|--------------------------|---|
| Course Title/Code | Drug Design and Drug Discovery (CHH618-T) |
| Course Type | Core |
| Course Nature | Elective |
| L-T-P-O Structure | 4-0-0-0 |
| Objectives | To familiarize with Principles of Drug design and drug discovery To impart knowledge on Quantitative Structure- Activity Relationship (QSAR) studies |
| Outcome | Students will be able to understand Principles of Drug design and drug discovery The student would be to understand Quantitative Structure- Activity Relationship (QSAR) studies and Combinatorial Synthesis |
| Prerequisites | Organic Chemistry-I & II |

| Syllabus | Sections | Weightage |
|----------|----------|-----------|
| | A | 25% |
| | B | 25% |
| | C | 25% |
| | D | 25% |
| | TOTAL | 100% |

SECTION-A

PRINCIPLES OF DRUG DESIGN AND DRUG DISCOVERY

Introduction to drug discovery. Folklore drugs, stages involved in drug discovery- disease, drug targets, bioassay. Discovery of a lead- screening of natural products and synthetic compound libraries, Existing drugs as leads (me too drugs). Pharmacokinetics (ADME), pharmacodynamics, Nature of drug – receptor interactions and their theories – Occupancy theory, Induced – fit theory, Macromolecular perturbation theory and Two-state model of receptor activation, Natural products as lead structures in drug discovery – Pharmacophore - structure

pruning technique e.g. morphine, Discovery of lead structure from natural hormones and neurotransmitters, Principles of design of agonists (e.g. Salbutamol), antagonists e.g. cimitidine) and enzyme inhibitors (e.g. captopril). Drug discovery without lead – serendipity- Penicillin and Librium as examples, Principles of prodrug design, Introduction to drug patents and Clinical trials.

SECTION-B

LEAD MODIFICATION AND SAR STUDIES

SAR: Lead modification strategies, Bioisosterism, variation of alkyl substituents, chain homologation and branching, variation of aromatic substituents, extension of structure, ring expansion and ring contraction, ring variation, variation and position of hetero atoms, ring fusion, simplification of the lead, rigidification of lead. Discovery of oxamiquine, salbutamol, cimitidine and captopril Structure-Activity Relationship studies in sulfa drugs, OC-26: Lead modification and SAR Studies

SECTION-C

QUANTITATIVE STRUCTURE- ACTIVITY RELATIONSHIP (QSAR) STUDIES

Introduction, physicochemical properties - pKa, electronic effects and Hammett constants(σ), lipophilicity constant(π), steric effects and Taft's constant, linear and nonlinear relationship between biological activity and Hammett/ Lipophilicity Substituent constants, Lipinski rule of five. Hansch analysis, Craig's plot, Topliss scheme, Free Wilson approach, cluster significant analysis, three case studies. Principles of molecular modeling in drug design.

SECTION-D

COMBINATORIAL SYNTHESIS INTRODUCTION: Combinatorial approach, Combinatorial libraries, technologies. Solid phase synthesis, types of resins. Linkers, Reactants for solid phased synthesis, Methods of Parallel synthesis: Haughton's tea bag procedure, Automated parallel synthesis, Methods in Mixed combinatorial synthesis: general principles. Furkas mix and split combinatorial synthesis, Structure determination of active compounds-Deconvolution, Methods in deconvolution recursive deconvolution, tagging and use of decoded

sheets, Examples of Combinatorial Chemistry, Planning and designing of combinatorial synthesis, Spider like scaffolds, drug molecules, Automation in Combinatorial chemistry, High throughput screening.

Books Recommended

1. Burger's medicinal chemistry and drug discovery by Manfred E. Wolf.
2. Patrick, Introduction to Medicinal chemistry.
3. R Silverman, Introduction to drug design.

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|--------------------------|---|
| Course Title/Code | PHOTOCHEMISTRY AND PERICYLIC REACTION (CHH619-T) |
| Course Type | Core |
| Course Nature | Hard |
| L-T-P-O Structure | 4-0-0-0 |
| Objectives | The student will be exposed to photochemistry of various electronic transitions The student will be introduced to various pericyclic reactions and their mechanisms |
| Outcome | The student will be able to write mechanism of various pericyclic reactions. Student will understand photochemistry of various electronic transition ($\pi\text{-}\pi^*$ and $n\text{-}\pi^*$) |
| Prerequisites | Organic Chemistry-I & II |

| Syllabus | Sections | Weightage |
|----------|----------|-----------|
| | A | 25% |
| | B | 25% |
| | C | 25% |
| | D | 25% |
| | TOTAL | 100% |

SECTION-A

PHOTOCHEMISTRY OF (π - π^*) TRANSITIONS: Excited states of alkenes, cis-trans isomerisation, photostationary state, electrocycloaddition and sigmatropic rearrangements, di- π methane rearrangement. Intermolecular reactions, photo cycloadditions, photodimerisation of simple and conjugated olefins, addition of olefins to α , β -unsaturated carbonyl compounds, excited states of aromatic compounds, Photoisomerisation of benzene

SECTION-B

PHOTOCHEMISTRY OF (n - π^*) TRANSITIONS: Excited states of carbonyl compounds, homolytic cleavage of α -bond, Norrish type I reactions in acyclic and cyclic ketones and strained cycloalkanediones, Intermolecular abstraction of hydrogen: photoreduction - influence of temperature, solvent, nature of hydrogen donor and structure of the substrate Intramolecular abstraction of hydrogen: Norrish type II reactions in ketones, Esters and 1, 2- diketones, Addition to carbon-carbon multiple bonds, Paterno-Buchi reaction, Photochemistry of nitrites-Barton reaction.

SECTION-C

PERICYCLIC REACTIONS I INTRODUCTION - Characteristics and classification of pericyclic reactions— Electrocyclic, cycloaddition & cycloreversions and sigmatropic reactions— $4n$ e and $4n+2$ e type examples, Approaches for the interpretation of mechanism of pericyclic reactions-Aromatic Transition States (ATS)/Perturbation, Molecular Orbitals (PMO) approach-Concept of Huckel –Möbius aromatic and antiaromatic transition states, Framing Woodward-Hofmann selection rules for all the pericyclic reactions by ATS approach, Solving problems based on ATS approach.

SECTION-D

PERICYCLIC REACTIONS II

Molecular orbitals-definition and their origin-Non-mathematical writing up of molecular orbitals and their symmetry properties for acyclic conjugated systems, Frontier Molecular Orbital (HOMO LUMO) approach-concept-Framing Woodward-Hofmann selection rules for all the pericyclic reactions by Frontier Molecular Orbital (FMO) approach, Solving problems based on FMO approach, Conservation of orbital symmetry (Correlation Diagrams) approach-concept- Framing Woodward-Hofmann selection rules for electrocyclic and cycloadditions & cycloreversions by Conservation of orbital symmetry approach.

Books Recommended

1. Mukherjee S M, Pericyclic Reactions
2. S. Sankararaman Pericyclic Reactions- A text Book, Wiley VCH, 2005
3. RM Silverstein, G C Bassler and T B Morrill Spectroscopic identification of organic compounds
4. William Kemp, Organic Spectroscopy
5. William Horsepool, Photochemistry

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| Course Title/Code | LABORATORY WORK-III (CHH620-P) |
| Course Type | Core |
| Course Nature L-T-P-O Structure | Hard 0-0-6-0 |
| Objectives | To familiarize with synthesis of organic compounds |
| Outcome | The student will be able to understand isolation of natural products |
| Prerequisites | Organic Chemistry-I & II |

SYNTHESIS OF ORGANIC MOLECULES & ISOLATION OF NATURAL PRODUCTS

Laboratory synthesis of the organic compounds such as

1. Preparation and characterization of two and three steps organic compounds.
2. Isolation of caffeine from tea leaves
3. Isolation of piperine from black pepper
4. Isolation of β carotene from carrots

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| Course Title/Code | LABORATORY WORK-IV (CHH621-P) |
| Course Type | Core |
| Course Nature | Hard |
| L-T-P-O Structure | 0-0-6-0 |
| Objectives | To familiarize with Multistage synthesis. To impart knowledge on isolation of natural products. |
| Outcome | The students will be able to understand enzymatic reaction and application of phase transfer catalysis |
| Prerequisites | Organic Chemistry-I & II |

1. Multistage synthesis including photochemical and enzymatic methods (some example given below)
 - a. Benzophenone-Benzapinacol-Benzapinacolone
 - b. Bezoin-benzil-benzilic acid
 - c. Cyclohexanone-cyclohexanone-caprolactone
2. Enzymatic reaction: reduction of ethyl acetoacetate with Baker yeast's, PPL catalyses deacetylation of 2-4 diacetoxy acetophenone
3. Application of Phase transfer catalysis in organic synthesis

Recommended Books:

1. Vogel Practical Organic Chemistry.

2. R K Meckie, D M Smith & R A Atken .Guidebook to organic synthesis
3. Micheal B Smith, Organic Synthesis
4. Fieser & Fieser, Organic synthesis, Vol 1-11 (1984)
5. Robert E Ireland, Organic synthesis
6. Reich and Rigby, Handbooks of reagents for organic synthesis Vol-I-IV

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|--------------------------|---|
| Course Title/Code | Seminar (CHN622) |
| Course Type | Core |
| Course Nature | Hard |
| L-T-P-O Structure | 0-0-0-2 |
| Objectives | To impart understanding of research papers/articles in specific areas To improve the communication skills by presentation on specific subjects |

SEMSETER IV

| COURSE CODES | COURSE NAME | COURSE TYPE | COURSE NATURE | PERIODS | | | | NO. OF CONTACT HOURS PER WEEK | CREDITS |
|--------------|---------------------------------|---|---------------------------------|---------|---|---|---|-------------------------------|---------|
| | | Core(Departmental/Allied)/ Elective (Departmental/ Open) / University Compulsory | Hard/Soft/ Workshop/ NTCC | L | T | P | O | | |
| CHH623-T | ADVANCED HETEROCYCLIC CHEMISTRY | CORE(Departmental) | HARD | 4 | 0 | 0 | 0 | 4 | 4 |

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| CHH624-T | CHEMISTRY OF NATURAL PRODUCTS | CORE(Departmental) | HARD | 4 | 0 | 0 | 0 | 4 | 4 |
| CHH625-T CHH626-T | ELECTIVE-II (A) BIOORGANIC CHEMISTRY (B) GROUP THEORY AND ITS APPLICATIONS | ELECTIVE(Departmental) | HARD | 4 | 0 | 0 | 0 | 4 | 4 |
| CHH627-P | LABORATORY WORK-V | CORE(Departmental) | HARD | 0 | 0 | 6 | 0 | 6 | 3 |
| CHN628 | PROJECT WORK | CORE(Departmental) | NTCC | 0 | 0 | 0 | 6 | 6 | 6 |

**DETAILED SYLLABUS
CHP01 –FOURTH SEMESTER**

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| Course Title/Code | ADVANCED HETEROCYCLIC CHEMISTRY (CHH623-T) |
| Course Type | Core |
| Course Nature L-T-P-O Structure | Hard 4-0-0-0 |
| Objectives | To impart knowledge on synthesis of Five and six- member heterocyclic compounds with two or more hetero atoms To familiarize with the synthesis of larger ring heterocyclic compounds |
| Outcome | Students will be able to write the synthesis of Five and six- member heterocyclic compounds with two or more hetero atoms Students will be able to write the synthesis of larger ring heterocyclic compounds |
| Prerequisites | Organic Chemistry-I & II |

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| Syllabus | Sections | Weightage |
| | A | 25% |

| | | |
|--|-------|------|
| | B | 25% |
| | C | 25% |
| | D | 25% |
| | TOTAL | 100% |

SECTION-A

NON-AROMATIC HETEROCYCLICS: Different types of strains, interactions and conformational aspects of nonaromatic heterocycles. Synthesis, reactivity and importance of the following ring systems, Azirines, Aziridines, Oxiranes, Thiiranes, Diazirenes, Diaziridines, Oxaziridines, Azetidines, Oxetanes and Thietanes

SECTION-B

FIVE AND SIX MEMBERED HETEROCYCLICS WITH TWO HETERO ATOMS: Synthesis, reactivity, aromatic character and importance of the following heterocycles: Pyrazole, Imidazole, Oxazole, Thiazole, Isoxazole, Isothiazole, Pyridazine, Pyrimidine. Pyrazine, Oxazine, thiazine, benzimidazole, benzoxazole and benzthiazole.

SECTION-C

HETEROCYCLICS WITH MORE THAN TWO HETERO ATOMS: Synthesis, reactivity, aromatic character and importance of the following Heterocycles: 1,2,3-triazoles, 1,2,4-triazoles, Tetrazoles, 1,2,4-oxadiazole, 1,3,4-oxadiazole, 1,2,5-oxadiazole, 1,2,3-thiadiazoles, 1,3,4-thiadiazoles, 1,2,5-thiadiazoles, 1,2,3-triazine, 1,2,4-triazine, 1,3,5-triazine, tetrazines. Synthesis and importance of purines and pteridines. Synthesis of Caffeine, theobromine and theophylline.

SECTION-D

LARGER RING AND OTHER HETEROCYCLICS: Synthesis, structure, stability and reactivity of Azepines, Oxepines and Thiepinines. Synthesis of Diazepines rearrangements of 1,2-diazepines. Synthesis of Benzoazepines, Benzodiazepines, Benzooxepines, Benzothiepinines, Azocines and Azonines. Synthesis of selenophenes, Tellerophenes, Phospholes and Boroles.

Books Recommended

1. T. Gilchrist, Heterocyclic Chemistry
2. R. M. Acheson, An introduction to the Chemistry of heterocyclic compounds

3. J.A.Joule & K.Mills, Heterocyclic Chemistry.
4. A.Paquette, Principles of Modern Heterocyclic Chemistry
5. J,A.Joule & , Heterocyclic Chemistry
6. A.R.Katritzky, Handbook of Heterocyclic Chemistry

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|--------------------------|---|
| Course Title/Code | CHEMISTRY OF NATURAL PRODUCTS (CHH624-T) |
| Course Type | Core |
| Course Nature | Hard |
| L-T-P-O Structure | 4-0-0-0 |
| Objectives | To impart knowledge on Biosynthesis of natural products.To familiarize with Structure determination and stereochemistry of natural products by chemical methods and spectroscopic methods |
| Outcome | Students will be able to write Biosynthesis of natural products.Students will be able elucidate the structure of natural products by various spectroscopic techniques |
| Prerequisites | Nil |

| Syllabus | Sections | Weightage |
|----------|----------|-----------|
| | A | 25% |
| | B | 25% |
| | C | 25% |
| | D | 25% |
| | TOTAL | 100% |

SECTION-A

PROTEINS: Biosynthesis of secondary metabolites: Introduction, Difference between Laboratory synthesis and biosynthesis. Methods for determination of biosynthetic mechanism. Isolation and identification of Biosynthetic precursors, Feeding experiments – use of radioisotopes Measurement of incorporation – absolute incorporation, specific incorporation, Identification of the position of labels in labeled natural products by chemical degradation and spectral methods. Major biosynthetic pathways: 1) Acetate-Malonate pathway: Biosynthesis of aromatic compounds, 2) Shikimic acid pathway ; Biosynthesis of essential amino acids – phenylalanine, tyrosine

and tryptophan, carboxylic acid derivatives, flavonoids and morphine alkaloids, 3) Mevalonic acid pathway : Biosynthesis of terpenes – mono, sesqui, di, tri (β -amyrin) and carotenoids, steroids – cholesterol.

LIPIDS: Lipid structure- acylglycerols, phosphoglycerides and sphingolipids, Biosynthesis of Lipids and chemical Synthesis of lipids.

SECTION-B

Terpenoids: Classification, nomenclature, occurrence, isolation, general methods of structure determination, isoprene rule. Structure determination, biosynthesis and synthesis of the following representative molecules: Monoterpenoids: Citral, geraniol (acyclic), α -terpeneol, menthol (monocyclic). Sesquiterpenoids: Farnesol (acyclic), zingiberene (monocyclic), santonin (bicyclic), Diterpenoids: Phytol and abietic acid.

Carotenoids and Xanthophylls: General methods of structure determination of Carotenes: β - carotene, α -carotene, γ - carotene, lycopene and vitamin A. Xanthophylls: Spirilloxanthin, Capsorubin, Fucoxanthin. Carotenoid acids (Apocarotenoids): Bixin and Crocetin. Bio synthesis of carotenoids.

SECTION-C

Alkaloids: Definition, nomenclature and physiological action, occurrence, isolation, general methods of structure elucidation, degradation, classification based on nitrogen heterocyclic ring, role of alkaloids in plants. Structure, synthesis and biosynthesis of the following: Ephedrine, Coniine, Nicotine, Atropine, Quinine and Morphine.

SECTION-D

Steroids: Occurrence, nomenclature, basic skeleton, Diel's hydrocarbon and stereochemistry. Isolation, structure determination and synthesis of Cholesterol, Androsterone, Testosterone, Estrone, Progesterone. Biosynthesis of steroids

Plant Pigments: Occurrence, nomenclature and general methods of structure determination. Isolation and synthesis of Anthocyanins (Cyanin and pelargonidin), polyphenols: Flavones (chrysin), Flavonols (quercetin) and isoflavones (daidzein) coumarin, Quinones (lapachol), Hirsutidin. Biosynthesis of flavonoids: Acetate pathway and Shikimic acid pathway.

Books Recommended:

1. , J. Mann, R.S. Davidson, J. B. Hobbs, D.V. Banthrope and J. B. Harborne, Natural Products- Chemistry and Biological Significance, Longman, Essex.
2. I.L. Finar, ELBS Organic Chemistry Vol. II,.
3. M. Nogradi, Stereo selective synthesis- A Practical Approach VCH.
4. Ed. S. Coffey Rodd's Chemistry of Carbon Compounds, Elsevier
5. Ed. Kurt Hostettmann, M.P. Gupta and A. Marston. Chemistry, Biological and Pharmacological Properties of Medicinal Plants From the Americas , Harwood Academic Publishers.
6. B.A.Bohm, Introduction to Flavonoids, , Harwood Academic Publishers.
7. Atta-ur-Rahman M. I. Choudhary New Trends in Natural Product Chemistry, Harwood Academic Publishers.
8. Insecticides of Natural Origin, Sukh Dev, Harwood Academic Publishers.

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| Course Title/Code | BIOORGANIC CHEMISTRY (CHH625-T) |
| Course Type | Core |
| Course Nature L-T-P-O Structure | Elective 4-0-0-0 |
| Objectives | To familiarize with mechanism of enzymatic reactions. To impart knowledge on various enzymatic Models and transformation reactions To impart basic knowledge on Fermentation technology and genetic engineering |
| Outcome | Students would be able to understand various enzymatic models Students would be able to write various transformation reactions Students will be able to understand the basics of Fermentation technology and genetic engineering |
| Prerequisites | Organic Chemistry-I & II |

| Syllabus | Sections | Weightage |
|----------|----------|-----------|
| | A | 25% |
| | B | 25% |
| | C | 25% |
| | D | 25% |
| | TOTAL | 100% |

SECTION-A

ENZYMES AND THEIR ACTION

Introduction to enzymes. Transition state theory, Acid-Base catalysis, Covalent catalysis— Binding modes of catalysis (i) Proximity effect (ii) Transition state stabilization (iii) Strain and Distortion. Examples of some typical enzyme mechanisms for (1) Triose phosphate isomerase, (ii) α -chymotrypsin and serine protease (iii) Lysozyme (iv) Carboxy peptidase-A (v) Ribonuclease..

SECTION-B

ENZYME MODELS AND ENZYMATIC TRANSFORMATIONS

Introduction — Biomimetic chemical approach to biological systems-Enzyme models Advantage of enzyme models. Requirements necessary for the design of enzyme models, Host-Guest complexation chemistry. Examples of some host molecules-Crown ether cryptanes, cyclodextrins, Cyclodextrin based enzyme models-Valixarenes, ionophores, micelles and synzymes (synthetic enzymes) — chiral recognition and catalysis. Introduction to industrial enzymes, Enzymatic synthesis of α -amino acids and peptides, Transformations of lipases and esterases, Kinetic resolutions of carboxylic acids, esters and alcohols – Transesterification, Amine resolution-use of oxido-reductase, C-C bond formation using enzymes-asymmetric cyanohydrin formation and asymmetric aldol condensations.

SECTION-C

RECOMBINANT DNA AND FERMENTATION TECHNOLOGY

Introduction to genetic engineering. Recombinant DNA technology-restriction endonuclease, cloning, linkers, adaptors, Application of recombinant DNA technology in production of pharmaceuticals, diagnosis of diseases, insect control, improved biological detergents, gene therapy-examples, Principles of finger printing technology-Site directed mutagenesis,

FERMENTATION TECHNOLOGY: Introduction to fermentation. Industrial fermentation, Advantages and limitations of fermentation, Production of drugs and drug intermediates from fermentation examples, Chiral hydroxy acids, vitamins, amino acids, β -lactam antibiotics, Precursor fermentation and microbial oxidation and reductions.

SECTION-D

COENZYMES: Introduction, Co factors — cosubstrates — prosthetic groups. Classification — Vitamin derived coenzymes and metabolite coenzymes. Structure and biological functions of coenzyme, thiamine pyrophosphate (TPP), pyridoxal phosphate (PLP), oxidized and reduced forms of i) nicotinamide adenosine dinucleotide / their phosphates (NAD), NADH, NADP+ NADPH) ii) Flavin adenine nucleotide FAD, FADH₂ and iii) Flavin mononucleotide (FMN, FMNH₂) lipoic acid, biotin, tetrahydrofolate and ubiquinone, Adenosine triphosphate (ATP) and adenosine diphosphate (ADP), S-adenosyl methionine (SAM) and uridine diphospho sugars (UDP-sugars) Mechanism of reactions catalyzed by the above coenzymes.

Recommended Books

1. D. Balasubramanian, Concepts in biotechnology
2. Horton, Principles of biochemistry
3. Herman Dugas and Christopher Penney Bioorganic chemistry - A chemical approach to enzyme action.
4. R.Sheldon Chirotechnology by Lymphoma Kinase (ALK) Martin P. Edwards, J. Med. Chem., 2011, 54 (18), pp 6342 6363.

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|--------------------------|---|
| Course Title/Code | GROUP THEORY AND ITS APPLICATIONS (CHH626-T) |
| Course Type | Core |
| Course Nature | Elective |
| L-T-P-O Structure | 4-0-0-0 |

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| Objectives | To familiarize with Symmetry elements and symmetry operations To impart knowledge on optical activity |
| Outcome | Students will be able to understand group representation of various molecules. |
| Prerequisites | Organic Chemistry-I & II |

Section A

MOLECULAR SYMMETRY: Symmetry elements and symmetry operations, definition of group and its characteristics, subgroups, classes, similarity transformation. Products of symmetry operations, equivalent atoms and equivalent symmetry elements, relations between symmetry elements and operations, classes of symmetry operations, point groups and classification. Symmetry: Optical activity and dipole moment

Section B

REPRESENTATION OF GROUPS: Reducible and irreducible representations. The great Orthogonality theorem, character tables, position vector and base vector as basis for representation. Wavefunctions as bases for irreducible representations (p and d-orbitals). Direct product. Vanishing integral.

Section C

COUPLING FOR TRANSITION METALS: Russell-Saunders coupling for d_n method of states. Splitting of one-electron levels in an octahedral environment. Correlation diagram. The method of descending symmetry, selection rules.

Section D

APPLICATION OF GROUP THEORY: Applications of group theory in Vibrational Spectroscopy: A brief idea about Infrared and Raman scattering spectroscopy. Vibrational modes as basis of group representations w.r.t. SO_2 , $POCl_3$, $PtCl_4^{2-}$ and RuO_4 . Mutual exclusion principle, Classification of vibrational modes (i.e. stretching and angle deformation vibrations w.r.t. SO_2 , $POCl_3$ and $PtCl_4^{2-}$).

Books Recommended

1. F.A.Cotton, Chemical applications of Group Theory
2. Durrant and Durrant, Inorganic Chemistry
3. Jaffe and Orchin, Symmetry in Chemistry

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| Course Title/Code | LABORATORY WORK-V (CHH627-P) |
| Course Type | Core |
| Course Nature L-T-P-O Structure | Hard 0-0-6-0 |
| Objectives | To familiarize with synthesis of drugs in laboratory To impart knowledge on estimation of drugs. |
| Outcome | Students will be able to understand synthesis of drugs in laboratory and their estimation. |
| Prerequisites | Organic Chemistry-I & II |

(A) LABORATORY SYNTHESIS OF THE FOLLOWING DRUGS:

Paracetamol, Phenytoin, Benzocaine, 6-Methyluracil, Chloritone, 4-Aminobenzene sulfonamide, Fluorescien and antipyrine.

(B DRUG ANALYSIS:

Aspirin (titrimetry), Ibuprofen (titrimetry), Analgin (titrimetry), Chloride in Ringer's lactate (argentometry), ascorbic acid {titrimetry, Iodometry and Cerimetry}, colorimetry}, Isoniazid(Iodometry), Riboflavin(colorimetry).

Books Recommended

1. Mann & Saunders, Practical organic chemistry
2. Vogel, Text book of practical organic chemistry

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|--------------------------|------------------------------|
| Course Title/Code | Project Work (CHN628) |
| Course Type | Core |
| Course Nature | Hard |

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|--------------------------|---|
| L-T-P-O Structure | 0-0-0-6 |
| Objectives | To make the students understand and analyze the specific problem To plan the experimental work and analyze the results To compile the data and prepare the project report |