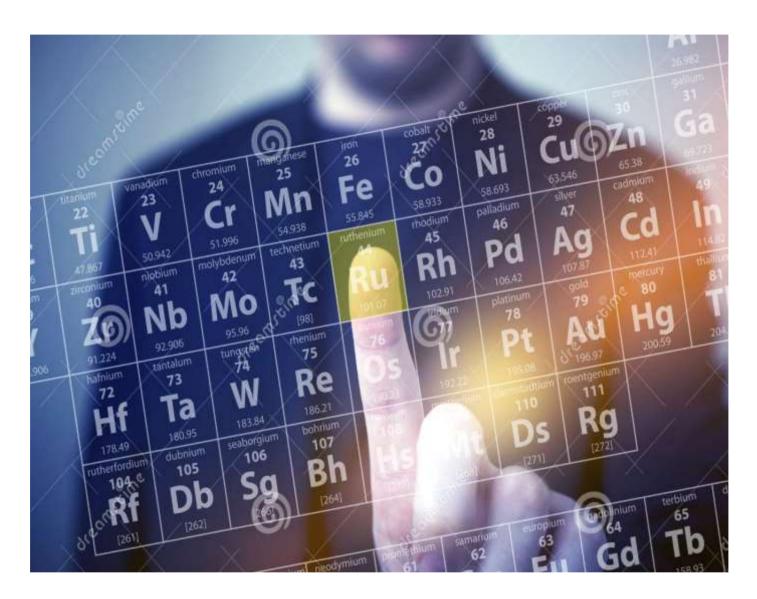


### **CHAITANYA DEGREE & PG COLLEGE FOR WOMEN**

Affiliated to Andhra University, Chaitanya nagar, Old Gajuwaka, Visakhaptnam-530026.

# DEPARTMENT OF CHEMISTRY



# M.Sc., ORGANIC CHEMISTRY LESSON PLANS



### **Academic-Pedagogical-Evaluation: Course Overview**

|          | P1  | Lecture             |
|----------|-----|---------------------|
|          | P2  | Demonstration       |
|          | Р3  | Question & Answer   |
| Pedagogy | P4  | Debate              |
|          | P5  | Audio & video clips |
|          | PQ  | Quiz                |
|          | PT  | Test                |
|          | P10 | Seminar             |
|          | PI  | Invited Lecture     |

### **SEMESTER - I**

### PAPER -I: GENERAL CHEMISTRY – I

| Course: M.Sc., (Organic Chemistry) | Year/Semester  | r: 1-1 Fa                   | aculty Name: <b>F</b> | 3.Leela kumar | i        |
|------------------------------------|--|-----------------------------|-----------------------|---------------|----------|
| Subject                            | PAPER-1: GENERAL CHEMISTRY-I   |                             |                       |               |          |
| <b>Units:</b>                      | <ul> <li>1.Rotational spectra of diatomic molecules</li> <li>2.Raman effect-classical and quantum mechanical explanations</li> <li>3.Spin Resonance Spectroscopy</li> <li>4.Basic concepts of Symmetry and Group theory</li> <li>5.Basic components of Computers, higher and lower level languages, Microsoft Fortran</li> </ul> |                             |                       |               |          |
| Learning<br>Objectives             | <ul> <li>Learn and understand the selection rules and criteria for molecules to exhibit rotational and IR spectroscopy.</li> <li>Understand the Classical and quantum mechanical theories of Raman spectroscopy and basic concepts of electronic spectroscopy.</li> </ul>  |                             |                       |               |          |
|                                    |  | spectrosco<br>ance principl | pic methods les.      | based on m    | nagnetic |
|                                    | <ul> <li>Learn basics of group theory and its application in chemistry.</li> <li>Understand the basic concepts of FORTRAN programming and its applications.</li> </ul>   |                             |                       |               |          |
| Units                              | U1   | U2                          | U3                    | U4            | U5       |
| Total Hours: 60                    | 12   | 12                          | 12                    | 12            | 12       |

| Internal   | $_{\it A}$ | $\Delta$ | 4 | $\it \Lambda$ | $\it \Delta$ |  |
|------------|------------|----------|---|---------------|--------------|--|
| Evaluation | 7          | 7        | 7 | 7             | 7            |  |

**Study materials (handouts)** 

http://www.nou.ac.in/econtent/Msc%20chemistry%20paper%202/MSc%20Chemistry%20Paper-II%20Unit-4.pdf

http://www.nou.ac.in/econtent/Msc%20Chemistry%20Paper%20IX/MSc%20Chemistry%20Paper-IX%20Unit-6.pdf

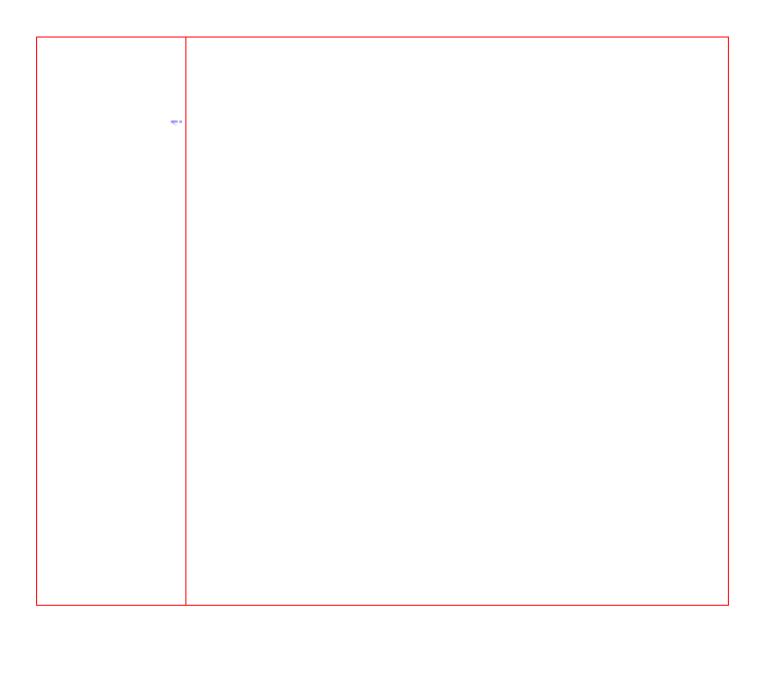
#### **Reference books:**

- 1. Symmetry and Spectroscopy of Molecules, K Veera Reddy, New Age International Publishers.
- 2. Physical Chemistry by Peter Atkins and Julio de Paula, Oxford University Press.
- 3. Chemical Applications of Group Theory, F. A. Cotton Wiley Eastern Limited New Delhi.
- 4. Group Theory and its Applications to Chemistry, K. V. Raman, Tata McGraw Hill Publishing Company Ltd., New Delhi.
- 5. Computer programming in Fortran-IV by V.Rajaraman, Prentice-Hall of India Pvt. Ltd., New Delhi.
- 6. Molecular Spectroscopy, Gordon M. barrow.
- 7. Fundamentals of Molecular Spectroscopy Banwell.

#### YouTube Links:

https://www.youtube.com/watch?v=3-8nAn0Mo6w

#### Model Question paper:



| UNIT | DESCRIPTION  | PEDAGOGY            | INTERNAL<br>EVALUATION |
|------|--|---------------------|------------------------|
| I    | 1.ROTATIONAL SPECTRA  Rotational spectra of diatomic molecules-rigid rotor- selection rules-calculation of bond length- isotopic effect, second order stark effect and its applications, Infrared spectra of diatomic molecules-harmonic and anharmonic oscillators. Selection rules-overtones- combination bands calculation of force constant, anharmonicity constant and zero point energy. Fermi resonance, simultaneous vibration rotation spectra of diatomic molecules.                               | P1,P3,P4,<br>P5,P10 | P10,PT                 |
|      | 2.RAMAN EFFECT-CLASSICAL AND QUANTUM MECHANICAL EXPLANATIONS   | P1,P3,P4,P<br>5,P10 | PQ,PT                  |
| п    | Raman effect-classical and quantum mechanical explanations-Rotational Raman and vibrational Raman spectra, Electronic spectra of diatomic molecules-Vibrational coarse structure-intensity of spectral lines-Franck Condon principle-applications, Rotational fine structure-band head and band shading, Charge transfer spectra.  |                     |                        |
|      | 3. SPIN RESONANCE SPECTROSCOPY   | P1,P3,P4,           | P10,PT                 |
| Ш    | Spin Resonance Spectroscopy: Principle and theory of NMR spectroscopy-Nature of spinning particle and its interaction with magnetic field. Chemical shift and its origin. Spin-Spin interaction- experimental methods. Application of NMR to structural elucidation-Structure of ethanol, dimethylformamide, styrene and acetophenoneri. Principle and theory of ESR-g-factor,   | P5,P10              |                        |
|      | hyperfine interactions-applications of ESR studies to  |                     |                        |
|      | the structure of free radicals, metal complexes.   |                     |                        |
| IV   | 4.CONCEPTS OF SYMMETRY AND GROUP THEORY Basic concepts of Symmetry and Group theory – Symmetry elements, symmetry operations and point groups – Schoenflies symbols – Classification of molecules into point groups – Axioms of Group theory – Group multiplication tables for C2V and C3V point groups –Similarity Transformation and classes – Representations – reducible and irreducible representations, Mulliken symbols, Orthogonality theorem and its implications, character table and its anatomy. | P1,P3,P4,P<br>5,P10 | PT,PQ                  |

| 5. BASIC COMPONENTS OF COMPUTERS, HIGHER AND LOWER LEVEL LANGUAGES, MICROSOFT FORTAN Basic components of Computers, higher and lower level languages, Microsoft Fortran: constants ariables and operators, arithmetic expressions, assignment and replacement statements, Input and Output statements — Format free and Format directed I/O statements — Iw, Fw.d, Ew.d and Gw.d format specifications, conditional and unconditional statements — Logical IF, Block IF an Go To statements, Do statement — syntax and rules. | 1 | PQ,PT |
|---|---|-------|
| Application of Chemical Problems:   |   |       |
| Flowcharts and Programs for   |   |       |
| <ol> <li>Statistical Analysis calculation of arithmetic mean, mean deviation, variance and standard deviation of replicate measurements.</li> <li>Solution of Quadratic equation – calculation of the roots of a quadratic equation.</li> </ol>   |   |       |
| 3. Calculation of the pH and hydrogen ion concentratio of an aqueous solution of a strong acid taking into account the auto ionization of water.  | n |       |
| 4. Calculation of the root of a polynomial using Gauss-Newton method – Application to Vander-Waal's equation.   |   |       |
| 5. Calculation of the rate constant of a first order reaction or calculation of molar extinction coefficient using Bee Lambert's Law by Linear least-squares method.  |   |       |

### **PAPER -II: INORGANIC CHEMISTRY – I**

| Course: M.Sc. (Organic Chemistry) | Year/Semesto   | er: 1-1 Fa  | culty Name: ( | CH, MALLIK | A  |  |
|-----------------------------------|--|---|---------------|------------|----|--|
| Subject                           | PAPER-II   | : INORGANI  | C CHEMISTRY   | '-I        |    |  |
| Units                             | <ol> <li>a. Inorg</li> <li>b. Poly</li> <li>Coordin</li> <li>Electro</li> <li>a. Tana</li> <li>tetrahe</li> </ol>  | <ol> <li>Structure &amp; Bonding</li> <li>a. Inorganic cage and ring compounds</li> <li>b. Polyacids</li> <li>Coordination compounds</li> <li>Electronic spectra of transition metal complexes</li> <li>a. Tanabe- Sugano diagrams for d1 –d9 octahedral and tetrahedral, transition metal complexes of 3d series.</li> <li>b. Magnetic properties of metal Complexes.</li> </ol> |               |            |    |  |
| Learning<br>Objectives            | <ul> <li>Acquire the knowledge on applications of VSEPR,         Valence Bond and Molecular orbital theories in         explaining the structures of simple molecules and role         of p and d orbitals in pi bonding.</li> <li>Understand the concept of MO theory to square planar         (PtCl4 2- ) and Octahedral complexes (CoF6 3- ,</li> </ul> |   |               |            |    |  |
|                                   | <ul> <li>Co(NH3)6 3+), and Walsh diagram for H2O molecule</li> <li>Apply the knowledge and understanding of         Understand the Orgel and Tanabe-Sugano diagrams         for d1 –d 9 octahedral and tetrahedral transition meta         complexes of 3d series to newly prepared         metal complexes     </li> </ul>                                |   |               |            |    |  |
|                                   | <ul> <li>Develop interest in the areas of magnetic properties of transition and inner transition metal complexes – spin and orbital moments – quenching of orbital momentum by crystal fields in complexes.</li> <li>To understand the concept of Term symbols and Electronic spectra and Magnetic properties of complexes.</li> </ul>                     |   |               |            |    |  |
| Units                             | U1   | U2  | U3            | U4         | U5 |  |

| Total Hours : 60       | 12 | 14 | 13 | 11 | 10 |
|------------------------|----|----|----|----|----|
| Internal<br>Evaluation | 4  | 4  | 4  | 4  | 4  |

#### **Study Material (Handouts):**

1. <a href="https://uomustansiriyah.edu.iq/media/lectures/6/6">https://uomustansiriyah.edu.iq/media/lectures/6/6</a> 2018 12 19!11 20 35\_PM.pdf

#### **Reference Books:**

- 1. Advanced Inorganic Chemistry by F.A. Cotton and G. Wilkinson, IV Edition, John Wiley and Sons, New York, 1980.
- 2. Inorganic Chemistry by J.E. Huheey, III Edition, Harper International

Edition, 1983.

3. Theoretical Inorganic Chemistry, II Edition by M.C. Day and J. Selbin,

Affiliated East-West press Pvt. Ltd., New Delhi.

4. Inorganic Chemistry by Shriver and Atkins, Oxford University Press (1999).

#### YouTube Links:

https://www.youtube.com/watch?v=XBdJY3JGJgA

#### **Power Point Presentations:**

- 1. <a href="https://docs.google.com/presentation/d/1UE5sR0eJh61IjEuB\_Z1svdIZVOv5orOb/edit#slide=id.p14">https://docs.google.com/presentation/d/1UE5sR0eJh61IjEuB\_Z1svdIZVOv5orOb/edit#slide=id.p14</a>
- 2. https://kanchiuniv.ac.in/coursematerials/Electronic%20spectra.pdf
- 3. https://uomustansiriyah.edu.iq/media/lectures/6/6 2018 12 19!11 20 35\_PM.pdf

#### **Model Question paper:**

| UNIT | DESCRIPTION  | PEDAGOGY            | INTERNAL<br>EVALUATION |
|------|--|---------------------|------------------------|
| I    | 1. STRUCTURE & BONDING Structure & Bonding: Applications of VSEPR, Valence Bond and Molecular orbital theories in explaining the structures of simple molecules- role of p and d orbitals in pπ-dπ bonding, Bent's rule, Non-valence cohesive forces. Application of MO theory to square planar (PtCl42-) and octahedral complexes (CoF63-, Co (NH3)63+). Walsh diagrams for linear (BeH2) and bent (H2O) molecules  | P1,P3,P4,<br>P5,P10 | P10,PT                 |
| II   | 2a. INORGANIC CAGE AND RING COMPOUNDS  Inorganic cage and ring compounds – preparation, structure and reactions of boranes, carboranes, metallocarboranes, Boron–Nitrogen (H3B3N3H3), Phosphorus–Nitrogen (N3P3Cl6) and Sulphur-Nitrogen (S4N4, (SN)x) cyclic compounds.  Structure and bonding in higher boranes with (special reference to B12 icosahedra). Electron counting rules in boranes – Wades rules (Polyhedral skeletal electron pair theory). | P1,P3,P4,<br>P5,P10 | PQ,PT                  |
|      | <b>2b. POLYACIDS</b> Polyacids:Introduction to polyacids- Types of polyacids- Isopolyacdis, Isopoly molybdates, Isopolytungstates, Isopolyvanadates, Structures of Polyacids [Mo <sub>7</sub> O <sub>24</sub> ] <sup>6-</sup> , [V10O28]6- and [W4O <sub>16</sub> ] <sup>8-</sup> , Heteropolyacids- properties of heteropolyacids and   |                     |                        |

|     | salts, structures of heteropolyacids and theories, Mialalicopause and Roscnneium theories, Pauling's theory and keggin's theory, applications of polyacids.  |                     |        |
|-----|--|---------------------|--------|
| III | 3. COORDINATION COMPOUNDS Coordination compounds: Crystal field theory - crystal field splitting patterns in octahedral, tetrahedral, tetragonal, square planar, square pyramidal and trigonal bipyramidal geometries. Calculation of crystal field stabilization energies. Factors affecting crystal field splitting energies – Spectrochemical series, Jahn – Teller theorem (static and dynamic Jahn-Teller theorem) and its consequences, nephelauxetic effect, applications and limitations of CFT; ligand field theory Experimental evidences for covalence in complexes. Molecular Orbital Theory of bonding for Octahedral, tetrahedral and square planar complexes. π-bonding and MOT-Effect of π - donor and π -acceptor ligands on Δo. Experimental evidence for π - bonding in complexes.            | P1,P3,P4,<br>P5,P10 | P10,PT |
| IV  | 4.ELECTRONIC SPECTRA OF TRANSITION METAL COMPLEXES Term symbol-Free Ion terms and Energy Levels: Configurations, Terms, States and Microstates, calculation of Microstates for P² and d2 Configuration, Russell- Saunders Coupling Schemes, J-J Coupling scheme, derivation of terms for various configurations P² and d² configuration, spectroscopic Ground state, Hole Formalism, Energy ordering of terms (Hund's Rules), Selection rules: Laporte orbital selection rule, spin selection rules. Splitting of energy levels and spectroscopic states Orgel diagrams of d1 to d9 metal complexes. Interpretation of electronic spectra of aquo Complexes of Ti(III), V(III), Cr(III), Mn(II), Fe(II), Fe(III), Co(II), Ni(II) and Cu(II). Calculation of interelectronic and spectral parameters for d8 metal | P1,P3,P4,<br>P5,P10 | PT,PQ  |
| V   | 5a. TANABE-SUGANO DIAGRAMS FOR d1-d9 OCTAHEDRAL AND TETRAHEDRAL METAL COMPLEXES OF 3d SERIES   | P1,P3,P4,<br>P5,P10 | PQ,PT  |

Tanabe- Sugano diagrams for d1 -d9 octahedral and tetrahedral transition metal complexes of 3d series. Calculation of Dq, Racah Parameter (B) and nephelauxetic parameter ( $\beta$ ), Charge transfer (L $\rightarrow$ M and M $\rightarrow$ L) spectra of metal complexes.

# 5b. MAGNETIC PROPERTIES OF METAL COMPLEXES

Magnetic properties of metal Complexes: Types of magnetic behavior, Temperature independent paramagnetism. Magnetic properties of transition and inner transition metal complexes – spin and orbital moments – quenching of orbital momentum by crystal fields in complexes. Magnetic susceptibility and its determination by Gouy's method, and Faraday's method. orbital contribution to magnetic moment (Oh and Td Complexes)

### **PAPER -III: ORGANIC CHEMISTRY – I**

| Course: M.Sc. (Organic Chemistry) | Year/Semester: 1-1 Faculty Name: R.Anuradha  |  |  |  |
|-----------------------------------|--|--|--|--|
| Subject                           | PAPER-III: ORGANIC CHEMISTRY-I   |  |  |  |
|                                   | <ol> <li>Aliphatic Nucleophilic Substitutions</li> <li>Aliphatic Electrophilic Substitutions</li> <li>Stereochemistry and conformational analysis</li> </ol> |  |  |  |
| Units                             | <ul><li>4. Chemistry of heterocyclic compounds</li><li>5. Chemistry of Natural Products</li></ul>  |  |  |  |

| Learning<br>Objectives | substitue and non  Understa  To know analysis  Develop compou  To acquir | ntion, neighborn-classical carrind aliphatic e about stereocs. interest in the ands. re knowledge | te of aliphatic ring group me bocations.  lectrophilic such emistry and area of chemistry and in the chemistry and steroids and of the chemistry and of the | chanism by ( bstitution reaconformation istry of hetero | actions.  nal  ocyclic |  |
|------------------------|--|---|---|---|------------------------|--|
| Units                  | U1   | U2  | U3  | U4  | U5                     |  |
| Total Hours : 60       | 14 9 13 12 12  |   |   |   |                        |  |
| Internal<br>Evaluation | 4  | 4   | 4   | 4   | 4                      |  |

#### **Study Material (Handouts):**

1. https://www.siue.edu/~tpatric/NS.pdf

#### **Reference Books:**

- 1.Advanced Organic Chemistry: Reactions Mechani;sms and Structure by Jerry March, Mc.Graw Hill and Kogakush.
- 2. Organic Chemistry Vol. I (Sixth Ed.) and Vol. II (Fifth Ed.) by I L Finar ELBS.
- 3. Organic Chemistry (fifth Ed., ) by Morrison and Boyd, PHI, India.
- 4. Organic Chemistry (fifth edition) by Francis A. Carey Tata Mc Graw Hill publishing Company Limited, New Delhi.
- 5. Stereochemistry of Organic compounds by Ernest L. Eliel, Samuel H. Wilen
- 6. Chemistry of natural products by S. V. Bhat, B. A. Nagasampangi and M. Siva kumar, Narosa Publishing House, 6th reprint, 2010

#### YouTube Links:

https://www.youtube.com/watch?v=yrvV85H7370

#### **Power Point Presentations:**

http://www.spcmc.ac.in/wp-content/uploads/2021/02/PPT-7P-Nucleophilic-Substitution-Reactions-1.pdf

#### **Model Question paper:**

| UNIT | DESCRIPTION  | PEDAGOGY            | INTERNAL<br>EVALUATION |
|------|--|---------------------|------------------------|
| I    | 1.ALIPHATIC NUCLEOPHILIC SUBSTITUTIONS The SN2, SN1, SNi and SET mechanisms. Substitution reactions of ambident nucleophiles, anchimeric assistance, the neighbouring group mechanism: neighbouring group participation by O, N, S, halogens, aryl groups, alkyl and cycloalkyl groups in nucleophilic substitution reactions. Sigma, Pi bond participation in acylic and bicyclic systems (Non- classic carbocations). Nucleophilic Substitution at allylic, trigonal and Vinylic carbons. Effect of substrate, attacking nucleophile, leaving group and reaction medium.   | P1,P3,P4,P<br>5,P10 | P10,PT                 |
| II   | 2.ALIPHATIC ELECTROPHILLIC SUBSTITUTIONS SE1, SE2, SEi Mechanisms: Reactivity-effects of substrate, leaving group and solvent. Reactions- hydrogen exchange, migration of double bonds, halogenation of aldehydes, ketones, carboxylic acids, acyl halides,  | P1,P3,P4,P<br>5,P10 | PQ,PT                  |
| III  | 3.STEREOCHEMISTRY AND CONFORMATIONAL ANALYSIS Optical isomerism: optical activity, molecular dissymmetry and chirality, elements of symmetry. Fischer's projection DL and RS configurations-relative and absolute configurations optical isomerism due to asymmetric carbon atoms-optical isomerism in Biphenyls, allenes and spiranes-optical isomerism of nitrogenous compounds, racemization and resolution. Geometrical isomerism: E,Z- configurations, properties of geometrical isomerism. Conformational analysis: conformations of acyclic molecules- alkanes and substituted alkanes, compounds having intramolecular hydrogen bonding. Conformations of cyclohexane, mono and disubstituted cyclohexane and decalins, effect of conformations on reactivity. | P1,P3,P4,P<br>5,P10 | P10,PT                 |
|      | 4. CHEMISTRY OF HETEROCYCLIC COMPOUNDS   | P1,P3,P4,P<br>5,P10 | PT,PQ                  |

| IV | Structure, reactivity and synthesis of reduced three membered heterocycles: (a) Oxirane: Sharpless method, Shi epoxidation, Jacobson epoxidation, etc (b) Aziridine; Four membered heterocycles: (a) Oxetane, Azetine; five membered heterocycles: (a) Pyrrole: Paul Knorr, Hantzsch methods,(b) Thiophene: Paul Knorr, Hinsberg methods, (c) Furan: Paul Knorr, Fiest- Benary, Industrial methods, etc, (d) Pyrazole, Imidazole, Oxazole, Thiazole; Six Membered Heterocycles: (a) Pyridine, Pyridazine, Pyrimidine and Pyrazine; Aromatic Heterocycles: (a) Indole; Fischer Indole synthesis, Bischler synthesis, Madelung synthesis, Domino and cascade method of Indole synthesis, (b) Quiniline and Isoquiniline, (c) Coumarins and Chromones. |                     |        |
|----|---|---------------------|--------|
| V  | 5. CHEMISTRY OF NATURAL PRODUCTS  A) Terpenoids: - Occurrence, Isolation, isoprene rule, structure elucidation and synthesis of α-Terpineol and α- pinene  B) Steroids:- Nomenclature of steroids, structure elucidation and synthesis and stereochemistry of cholesterol and progesterone  C) Lipids:- Classification, chemistry, properties and function-free fatty acids, triglycerides, phospholipids, glycolipids & waxes conjugated lipids-lipoproteins   | P1,P3,P4,P<br>5,P10 | P10,PT |

| Course: M.Sc., (Organic Chemistry) | Year/Semester:  | 1-1 Fa     | culty Name: B.L | eela Kumari |    |
|------------------------------------|---|------------|-----------------|-------------|----|
| Subject                            | PAPER-4:  | PHYSICAL ( | CHEMISTRY- I    |             |    |
| Units                              | 1.Thermodynamics-I 2.Thermodynamics-II 3.Surface Tension 4.Chemical Kinetics-I 5.Chemical Kinetics-II   |            |                 |             |    |
| Learning<br>Objectives             | <ul> <li>Explain the basic concepts of Thermodynamics and its applications</li> <li>Understand the concepts of thermodynamics of solutions.</li> <li>To understand the principle of micellisation.</li> <li>Understand the various kinetic theories, measurements of reaction rates.</li> <li>Learn experimental techniques for measuring the kinetics of fast reactions and</li> </ul> |            |                 |             |    |
| Units                              | U1  | U2         | U3              | U4          | U5 |
| Total Hours : 60                   | 12  | 11         | 13              | 12          | 12 |
| Internal<br>Evaluation             | 4   | 4          | 4               | 4           | 4  |

**Study Material (Handouts):** 

https://www.toppr.com/ask/content/posts/surface-chemistry/notes-28204/

#### Text Books:

- 1. Physical Chemistry by Peter Atkins and Julio de Paula, Oxford University Press.
- 2. Chemical Kinetics by K. J. Laidler, McGraw Hill Pub.
- 3. Physical chemistry by K.L. Kapoor

#### **Reference Books:**

- 1. Thermodynamics for Chemists, Samuel Glasstone
- 2. Physical chemistry by Puri, Sharma and Pathania
- 3. Micelles, Theoretical and applied aspects, V. Moroi, Plenum publisher

YouTube Links:

https://youtu.be/3ksUl-QGIDI

https://youtu.be/EqWJ7KIP04I

**Power Point Presentations:** 

https://web.iitd.ac.in/~sdeep/Thermo\_lecture\_4.ppt

Model Question paper:

|      | Unit - wise Plan Pedagogica   | II D valaati        |                        |
|------|---|---------------------|------------------------|
| UNIT | DESCRIPTION   | PEDAGOGY            | INTERNAL<br>EVALUATION |
| I    | 1. ThermoDynamics – I: Basic concepts of second law of Thermodynamics-Entropy- Entropy changes accompanying different processes-Entropy changes in an ideal gas, entropy changes in the mixing of ideal gases, entropy as a function of V and T and entropy as a function of P and T- Entropy change in isolated systems Clausius inequality- Helmholtz and Gibbs energy – Maxwell relations - Criteria for spontaneity-variation of Gibbs energy with temperature and pressure for solids, liquids and gases- Concept of fugacity-determination of fugacity coefficient of gases- Thermodynamics of phase transitions- Concept of chemical potential-Location of phase boundaries- (Clausius-Clapeyron equation for Liquid- Vapour, Solid -Liquid and Solid- Vapour boundaries)- Ehrenfest classification of phases. | P1,P3,P4,<br>P5,P10 | P10,PT                 |
| II   | 2. ThermoDynamics – II:  Thermodynamics of mixtures -partial molar quantities - experimental methods of determination of partial molar quantities - Gibbs-Duhem equation and Duhem-Margules equation-Thermodynamics of mixing of liquids (ΔHmix, ΔGmix and ΔSmix) - Thermodynamics of ideal solutions - Raoult's law - Thermodynamics of colligative properties of dilute solutions - concept of activity and activity coefficient-Experimental determination of activity coefficient - Thermodynamic concept of equilibrium, variation of equilibrium with temperature (Van't Hoff equation) and pressure - Nernst heat theorem, Third law of thermodynamics- exceptions to third law of thermodynamics.   | P1,P3,P4,<br>P5,P10 | P10,PT                 |

| III | 3. Surface tension:  Capillary action- Adsorption-Adsorption isotherms Freundlich adsorption isotherm,  Langmuir adsorption isotherm-limitations -  BET adsorption isotherm-estimation of  Surface area. Surface active agents,  classification of surface active agents,  micellization, hydrophobic interaction,  critical micellar concentration (CMC),  factors affecting the CMC of surfactants,  counter ion binding to micelles,  thermodynamics of micellization phase  separation and mass action models.   | P1,P3,P4,<br>P5,P10 | P10,PT |
|-----|--|---------------------|--------|
| IV  | 4. Chemical Kinetics- I:  Theories of reaction rates- Collision theory Limitations, Transition state theory. Lindeman's theory of unimolecular reactions- Limitations. Diffusion controlled reactions. Effect of ionic strength on rates of reactions- Primary and secondary salt effects. Effect of dielectric constant on reactions - kinetic isotope effect -Primary and secondary isotopic effects -Effect of substituent -Linear free energy relationships-Hamett equation - limitations- Taft equation. Kinetics of consecutive reactions, parallel reactions, opposing reactions (Uni molecular steps only, no derivation). | P1,P3,P4,<br>P5,P10 | PT,PQ  |
| V   | 5. Chemical Kinetics- II: Specific and general acid-base catalysis. Skrabal diagrams. Steady state approximation- Enzyme catalysis- Michaelis -Menten mechanism. Derivation of Kinetic equation and Kinetic parameters. Lock and Key hypothesis-pH dependence of enzyme catalyzed reactions. Fast reactions- different methods of studying fast reactions- flow methods, relaxation methods- temperature jump and pressure jump methods.   | P1,P3,P4,<br>P5,P10 | P10,PT |

### PAPER -I: GENERAL CHEMISTRY – II

| Course: M.Sc. (Organic Chemistry) | Year/Semester:  | 1-2 Fac   | culty Name: B.L | eela Kumari |    |
|-----------------------------------|---|-----------|-----------------|-------------|----|
| Subject                           | PAPER-1:  | GENERAL C | HEMISTRY-II     |             |    |
| Units                             | <ol> <li>Wave equation</li> <li>Wave mechanics of simple systems</li> <li>Hydrogen atom</li> <li>Variation principle</li> <li>Valence bond approach</li> </ol>  |           |                 |             |    |
| Learning Objectives               | <ul> <li>Students will have the idea of wave function and understand the uncertainty relations</li> <li>Students will learn how to solve the Schrodinger Eq. rigorously for model systems</li> <li>Students will be able to understand and be able to explain the origin of quantized energy levels</li> <li>Students will learn to apply concepts from physics and methods from mathematics to derive and understand the properties of chemical systems that arise from quantum mechanical models for the structure of atoms and molecules</li> <li>They will be able to understand and explain the</li> </ul> |           |                 |             |    |
| Units                             | differences between classical and quantum mechanics  U1 U2 U3 U4 U5   |           |                 |             |    |
| Total Hours : 60                  | 11  | 13        | 12              | 12          | 12 |

| Internal   | 4 | 4 | 4 | 4 | 4 |
|------------|---|---|---|---|---|
| Evaluation |   |   |   |   |   |

**Study Material (Handouts):** 

https://quantum.phys.cmu.edu/CQT/chaps/cqt02.pdf

YouTube Links: <a href="https://youtu.be/gNDnHWg-cDs">https://youtu.be/gNDnHWg-cDs</a>

https://youtu.be/jb8XvtEgAyk

**Power Point** 

Presentations: https://people.uleth.ca/~roussel/C2000/slides/08VBtheo

ry.pdf

Model Question paper:

http://www.nou.ac.in/econtent/Msc%20Chemistry%20Paper%20IX/

MSc%20Chemistry%20Paper-IX%20Unit-6.pdf

| UNIT | DESCRIPTION  | PEDAGOGY            | INTERNAL<br>EVALUATION |
|------|--|---------------------|------------------------|
| I    | 1. Wave equation: Interpretation of wave function – properties of wave function – normalization and orthogonalization, operators – linear and nonlinear commutators of operators, Postulates of quantum mechanics, setting up of operators observables – Hermitian operator – Eigen values of Hermitian operator.  | P1,P3,P4<br>,P5,P10 | P10,PT                 |
| П    | Wave mechanics of simple systems with constant potential energy, particle in one dimensional box – factors influencing colour – transition – dipole integral, symmetry arguments in deriving the selection rules-the concept of tunneling – particle in a three dimensional box, Rigid rotor, wave mechanics of systems with variable potential energy-simple harmonic oscillator solution of wave equation-selection rules. | P1,P3,P4,<br>P5,P10 | PQ,PT                  |
| III  | Hydrogen atom-solution of R(r), $\theta$ ( $\theta$ ) and $\Phi$ ( $\phi$ ) equations-probability density in orbitals-shapes of orbitals. Perturbation theory- time independent perturbation (only first order perturbation is to be dealt with) – application to ground state energy of hydrogen and helium atom  | P1,P3,P4<br>,P5,P10 | P10,PT                 |
| IV   | Variation principle-applications to hydrogen and helium atoms-calculation of zero point energy of harmonic oscillator-many electron atom-Comparison between Perturbation and variation theorems. Hartee-Fock self-consistent field method and introductory concepts of Density functional theory(DFT)  | P1,P3,P4<br>,P5,P10 | PT,PQ                  |
| V    | Valence bond approach-directed valence-hybridization-covalent bond calculation of ionic and covalent bond contributions in hydrogen molecule. Molecular orbital theory – LCAO approximation – hydrogen molecule ion – hydrogen molecule (fundamental concepts only) – The electronic transitions in the hydrogen molecule  | P1,P3,P4<br>,P5,P10 | PQ,PT                  |

| Course: M.Sc. (Organic Chemistry) | Year/Semester:   | 1-2 Fa                      | culty Name: CH      | . MALLIKA    |      |
|-----------------------------------|--|-----------------------------|---------------------|--------------|------|
| Subject                           | PAPER-II : INORGANIC CHEMISTRY-II  |                             |                     |              |      |
|                                   |  | cluster com<br>ometallic co | •                   |              |      |
|                                   | _  |                             | ilibria in solu     | ition:       |      |
| Units                             | 4. Determ comple   |                             | stability cons      | stants of    |      |
|                                   | 5. Reaction  | on Mechani                  | sms of Meta         | l Complexe   | es   |
|                                   | nd the definition  | on of clusters              | and                 |              |      |
| Learning                          | • Students are able to apply 18 and 16 electron rules to complexes to explain their stabilities.               |                             |                     |              |      |
| Objectives                        | <ul> <li>Students are able to understand the stability of<br/>complexes based on HSAB principle.</li> </ul>    |                             |                     |              |      |
|                                   | <ul> <li>Students will able to apply different methods to find<br/>stability constants in reaction.</li> </ul> |                             |                     |              | ind  |
|                                   |  | understand or mechanism     | lifferent reaction. | ons of compl | exes |
| Units                             | U1   | U2                          | U3                  | U4           | U5   |
| Total Hours : 60                  | 12 12 12 12  |                             |                     |              |      |
| Internal<br>Evaluation            | 4  | 4                           | 4                   | 4            | 4    |

#### **Study Material (Handouts):**

1. <a href="https://www.sscasc.in/wp-content/uploads/downloads/Chemistry/Inorganic-Chemistry.pdf">https://www.sscasc.in/wp-content/uploads/downloads/Chemistry/Inorganic-Chemistry.pdf</a>

 $\overline{\mathcal{M}}_{i}$ 

#### **Reference Books:**

- 1. Advanced Inorganic Chemistry by F.A. Cotton and R.G. Wilkinson, IV Edition, John, John Wiley and Sons, New York, 1980.
- 2. Inorganic Chemistry by J.E. Huheey, III edition, Harper International Edition, 1983.
- 3. Organometallic Chemistry-A unified approach by A. Singh and R.C. Mehrotra, Wiley Eastern Ltd.
- 4. Inorganic Chemistry by Shriver and Atkins, Oxford University Press (1999)
- 5. Theoretical Inorganic Chemistry, II Edition by M.C. Day and J. Selbin, Affiliated East-West press Pvt. Ltd., New Delhi.
- 6. Mechanisims of Inorganic reactions in solution by D.Benson, MCgraw Hill, London, 1968.
- 7. Inorganic chemistry by K.F. Purcell and J.C.Kotz, W.B. Saunders company, New York, 1977

#### YouTube Links:

https://www.youtube.com/watch?v=7gmAfRCDTk0

#### **Model Question paper:**

| UNIT   | DESCRIPTION   | PEDAGOGY            | INTERNAL<br>EVALUATION |
|--|---|---------------------|------------------------|
| Metal cluster compounds:  Definition – evidences for existence of M-M bonds - conditions favorable for formation of M-M bonds – preparation, structure and bonding of the following metal cluster compounds. Re2Cl8 2-, Mo2Cl8 4-, Re2(RCOO)4X2, Mo2(RCOO)4(H2O)2, Cu2(RCOO)4 (H2O)2, Cr2(RCOO)4 (H2O)2, Cr2Cl9 3-, Mo2Cl9 3-, W2Cl9 3-, Re3Cl9, Re3Cl123-, Mo6Cl8 4+, Nb6X122+ and Ta6X122+. Polyatomic clusters – Zintle ions, Chevrel phases. |   | P1,P3,P4,P5,<br>P10 | P10,PT                 |
| II   | Organometallic compounds:  16 and 18 electron rules., Isoelectronicrelationship - Synthesis, structure, bonding and reactions of carbon monoxide, dinitrogen and nitric oxide complexes. Isolobal relationship – H, Cl, CH3, Mn(CO)5; S, CH2, Fe(CO)4; P, CH, Co(CO)3 Synthesis, structure, bonding and reactions of metallocenes with special reference to ferrocene   | P1,P3,P4,<br>P5,P10 | PQ,PT                  |
| III  | Metal Ligand equilibria in solution:  Step wise and overall formation constants and their interaction. Trends in stepwise constants ((statistical effect and statistical ratio), factors affecting the stability of metal complexes; Stability correlations - Irwing -William's series, Pearson's theory of hard and soft acids and bases (HSAB), Application of HSAB: Biological functions and toxicology of metals, and medicinal applications; chelate effect and its thermodynamic origin | P1,P3,P4,<br>P5,P10 | P10,PQ                 |

|         | Determination of stability   | P1,P3,P4,           | PT,PQ |
|---------|--|---------------------|-------|
|         | constants of complexes:  | P5,P10              |       |
| IV      | Determination of stability constants of complexes by spectrophotometric method ((Job's method) and pH – metric method(Bjerrum's). Reactivity of metal complexes – inert and labile complexes. Explanation of lability on the basis of valence bond and crystal field theories. |                     |       |
|         | Reaction Mechanisms of Metal   | P1,P3,P4,<br>P5,P10 | PQ,PT |
|         | Complexes: Reactivity of metal   | 1 5,1 10            |       |
|         | complexes, inert and labile  |                     |       |
|         | complexes, Kinetics and mechanisms   |                     |       |
|         | of substitution reactions, kinetics of   |                     |       |
|         | substitutions reactions in octahedral  |                     |       |
|         | complexes, acid hydrolysis, Factors  |                     |       |
| ${f V}$ | affecting acid hydrolysis, Base  |                     |       |
|         | hydrolysis, Conjugate base mechanism, Anation reactions,   |                     |       |
|         | substitution reactions in square planar  |                     |       |
|         | complexes, Trans effect, Mechanism   |                     |       |
|         | of trans effect, Electron transfer   |                     |       |
|         | reactions— concept of complementary  |                     |       |
|         | and non-complementary reactions  |                     |       |
|         | with examples, inner sphere and outer  |                     |       |
| i       | sphere mechanisms, Marcus theory.  |                     |       |

### **PAPER -III: ORGANIC CHEMISTRY – II**

| Course: M.Sc., (Organic Chemistry) | Year/Semester:   | 1-2 Fac | culty Name: R. | ANURADHA |    |
|------------------------------------|--|---------|----------------|----------|----|
| Subject                            | PAPER-III: ORGANIC CHEMISTRY-II  |         |                |          |    |
| Units                              | 1.Aromaticity& Aromatic Nucleophilic Substitutions 2.Reactive Intermediates & Named Reactions 3.Molecular Rearrangements 4.Spectroscopy 5.Alkaloids & Peptides and Proteins & Nucleic acids  |         |                |          |    |
| Learning<br>Objectives             | <ul> <li>Acquire the knowledge of aromaticity, aromatic nucleophilic substitution</li> <li>Understand reactive intermediate and name reactions,</li> <li>Apply the knowledge and understanding of molecular rearrangements of electron deficient carbon, Nitrogen and Oxygen</li> <li>Develop interest in the areas of spectroscopy-Principles o9f UV, IR,NMR and Mass spectroscopy.</li> <li>To gain knowledge about alkaloids, peptides, proteins and nucleic acids</li> </ul> |         |                |          |    |
| Units                              | U1 U2 U3 U4 U5   |         |                |          |    |
| Total Hours : 60                   | 12   | 9       | 12             | 15       | 12 |

| Internal   | 4 | 4 | 4 | 4 | 4 |
|------------|---|---|---|---|---|
| Evaluation |   |   |   |   |   |

#### **Study Material (Handouts):**

https://courses.lumenlearning.com/suny-potsdamorganicchemistry/chapter/5-6-reactive-intermediates/

#### **Text books**

- 1. Organic Chemistry Vol. I (Sixth Edn.) and Vol. II (Fifth Ed.,) by IL finar ELBS.
- 2. Organic Chemistry (fifth Edn., ) by Morrison and Boyd, PHI, India.
- 3. Organic Chemistry (fifth edition) by Francis A. Carey Tata McGraw Hill publishing Company Limited, New Delhi.
- 4. Reaction Mechanism in Organic Chemistry by Mukherjee Sirigh, N Terniitarr, Indiar
- 5. A guide book to mechanism in Organic Chemistry by Peter Sykes, ELBS.

#### **Reference Books:**

- 1. Advanced organic chemistry by Jerry March (4th Edition)Wiley Eastern.
- 2. Stereochemistry of carbon compounds by E.Eliel, John Wiley & Sons, Inc.
- 3. Stereochemistry of Organic compounds by D. Nasipuri.
- 4. Chemistry of Natural products by R.S. KalsiKalyani Publishers. 1983

#### YouTube Links:

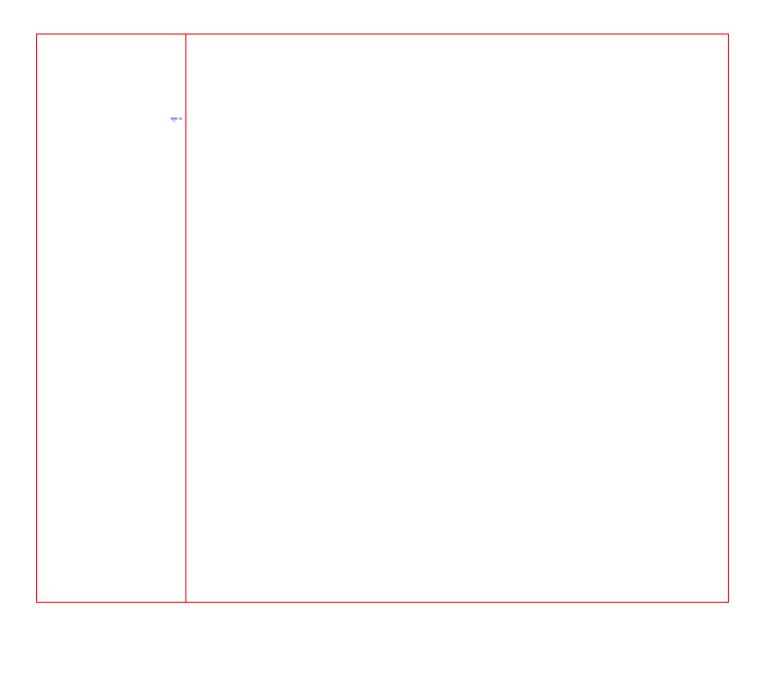
https://youtu.be/ZC8kp\_6Sd48

https://youtu.be/HhV3H-m5f2c

#### **Power Point Presentation:**

https://docs.google.com/presentation/d/1auI2BEKEwXSWPoMozMEZB8b NLjhZqyWB/edit#slide=id.p4

https://youtu.be/kaXeqpCYgX4
Model Question papers:



| UNIT | DESCRIPTION   | PEDAGOGY            | INTERNAL<br>EVALUATION |
|------|---|---------------------|------------------------|
| I    | <ul> <li>A) Aromaticity: Concept of Aromaticity, Aromaticity of five membered, six membered and fused systems -non-benzenoid aromatic compounds:- cyclopropenylcation, cyclobutadienyldication, cyclopentadienyl anion – tropyliumcation and cyclo octatetraenyl di anion – matallocenes, ferrocenes, azulenes, fulvenes, annulenes, fullerenes. Homo aromaticity, Anti aromaticity and Pseudo aromaticity.</li> <li>B) Aromatic Nucleophilic Substitutions: The SNAr, SN1, benzyne and SRN1 mechanisms. Reactivity: Effect of substrate, leaving group and attacking nucleophile. The Von- Richter ,Sommlet-Hauser and Smiles rearrangements.</li> </ul> | P1,P3,P4,<br>P5,P10 | P10,PT                 |
| II   | A) Reactive Intermediates:  Generation, structure, stability and reactivity of Reactive intermediates: carbanion, carbocation, free radicals, carbenes and nitrenes.  B) Named Reactions:  Wittig reaction, Grignard reaction, Stork enamine reaction, Michael addition, Mannich Reaction, Diel's-Alder reaction and Ene-reaction   | P1,P3,P4,<br>P5,P10 | PQ,PT                  |
| III  | Molecular Rearrangements:  Types of molecular rearrangements, migratory aptitude; Rearrangements to electron deficient carbon: Pinacol-pinacolone, Wagner-Meerweinand Benzil-Benzilic acid, Rearrangements to electron deficient nitrogen: Beckmann, Hofmann, Curtius, Schmidt and Lossen rearrangements; Rearrangements to electron deficient oxygen: Baeyer-villiger, Dakin rearrangements; Other rearrangements: Neber rearrangement and Favorskii rearrangements  | P1,P3,P4,<br>P5,P10 | P10                    |

| IV | A) UV Spectroscopy: Various electronic transitions, selection rules, effect of solvent on electronic transitions, the absorption laws, chromophores, auxochromes, bathochromic and hypso chromic shifts, hyperchromic and hypochromic effects, Woodward-Fieser rules for conjugated dienes and carbonyl compounds. B) Infrared Spectroscopy: Basic principles: types of molecular vibrations, fingerprint region and identification of functional groups. C) Nuclear Magnetic Resonance Spectroscopy (1H-NMR): nuclear spin, nuclear resonance, saturation, shielding of magnetic nuclei, chemical shifts, factors affecting the chemical shift, and assignment of chemical shifts. D) Mass Spectroscopy: Basic principles, nitrogen rule and fragmentation pattern of carbonyl compounds and alcohols | P1,P3,P4,<br>P5,P10 | PT,PQ |
|----|--|---------------------|-------|
| V  | A) Alkaloids:  Occurrence, Isolation, classification based on nitrogen heterocyclic ring and synthesis of quinine and nicotine B) Peptides and Proteins: α-Aminoacids, their general properties and synthesis, Synthesis of peptides by Merrifield solid phase synthesis.Primary, secondary and tertiary structures of proteins C) Nucleic acids: Heterocyclic bases; Purines: Adenine and Guanine; Pyramidines: Cytosine, Uracil and Thymine; nucleosides, nucleotides Basic concepts of the structures of RNA and DNA  | P1,P3,P4,<br>P5,P10 | PQ,PT |

### **PAPER -IV: PHYSICAL CHEMISTRY – II**

| Course: M.Sc., (Organic Chemistry) | Year/Semester:   | 1-2 Fac | culty Name: B.L | eela Kumari |    |  |
|------------------------------------|--|---------|-----------------|-------------|----|--|
| Subject                            | PAPER-IV: PHYSICAL CHEMISTRY-II  |         |                 |             |    |  |
| Units                              | 1.Crystal structure of solids 2.Classification of polymers 3.Electrochemistry I 4.Electrochemistry II 5.Photochemistry   |         |                 |             |    |  |
| Learning<br>Objectives             | <ul> <li>Explain the basic concepts of Crystallography</li> <li>Understand the types of polymers and analyze various physical properties of polymers</li> <li>Understand the concepts of electrochemistry and theories like Debye Huckel theory</li> <li>Understand the basic concept and theories of electrode-electrolyte interface</li> <li>Learn principles of photochemistry and various photochemical reactions</li> </ul> |         |                 |             |    |  |
| Units                              | U1   | U2      | U3              | U4          | U5 |  |
| Total Hours : 60                   | 12   | 12      | 12              | 12          | 12 |  |
| Internal<br>Evaluation             | 4  | 4       | 4               | 4           | 4  |  |

### **Study Material (Handouts):**

https://www.arsdcollege.ac.in/wp-content/uploads/2020/04/Glass-transition-Temperature-and-factors-affecting-1.pdf

140

### **Reference Books:**

- 1. Physical Chemistry by Peter Atkins and Julio de Paula, Oxford University Press
- 2. Physical Chemistry by G.W. Castellon, Narosha Publishing House
- 3. Physical chemistry by K.L. Kapoor.
- 4. Principles of photochemistry, RohitgeeMukhargee

### YouTube Links:

https://youtu.be/5h5gXoFyo64

### **Power Point Presentations:**

https://www.chemistry.mcmaster.ca/~aph/chem1a3/lectures/lec12/lec12.ppt Model Question paper:

http://www.nou.ac.in/econtent/Msc%20Chemistry%20Paper%20IX/MSc%20Chemistry%20Paper-IX%20Unit-6.pdf

| UNIT | DESCRIPTION  | PEDAGOGY                | INTERNAL<br>EVALUATION |
|------|--|-------------------------|------------------------|
| I    | Crystal structure of solids: Fundamental of lattices, unit cell, Bravais lattices, symmetry elements in crystals, packing efficiency, radius ratios; Miller indices. Structures and types of solids. Structure determination by X-ray diffraction (Bragg's equation). Magnetic properties of solids-Classification of magnetic materials, Magnetic susceptibility, Measurement of magnetic susceptibility. Electric properties- Band theory, the band structure of metals, insulators, and semiconductors. The temperature dependence of the conductivity of extrinsic semiconductors. Superconductivity and occurrence. Meisner effect. Types of superconductors. Theories of superconductivity - BCS theory. | P1,P3,<br>P4,P5,<br>P10 | P10,PT                 |
| II   | Classification of polymers:  Free radical, ionic and Zeigler - Natta Polymerization - kinetics of free radical polymerization - Techniques of polymerization - Glass transition temperature - Factors influencing the glass transition temperature - Number average and Weight average, Molecular weights - molecular weights determination - End group analysis - Osmometry - Light scattering and ultra-centrifugation methods.  | P1,P3,<br>P4,P5,<br>P10 | PQ,PT                  |
| III  | Electrochemistry I:  Ionic mobilities and conductivities - Debye-Huckel theory of strong electrolytes, Debye-Huckel onsagar equation- limitations- mean activity coefficient- Verification of Debye-Huckel limiting law. Electro chemical cell- Galvanic and electrolytic cell. Nernst equation- Concentration cell with and without transference- effect of complexation on redox potential- ferricyanide/ ferrocyanide couple, Iron (III) phenonthroline/ Iron(II) phenonthroline couple. Fuel Cells-  | P1,P3,<br>P4,P5,<br>P10 | P10,PT                 |

|    | constructionVarious types-Examples.  |                         |       |
|----|--|-------------------------|-------|
|    | Electrochemistry II:   | P1,P3,<br>P4,P5,        | PT,PQ |
| IV | The electrode-electrolyte interface. The electrical double layer. The Helmholtz-Perrin parallel-plate model, the Gouy-Chapman diffuse-charge model and the Stern model. Electrodics: Charge transfer reactions at the electrode-electrolyte interface. Derivation of Butler-Volmer equation. High field approximation, Tafel equation, Low field equilibrium, over voltage. Theories of over voltage-Corrosion - Concentration polarization - Polarography -Half wave potential and Ilkovic equation.  | P10                     |       |
| V  | Photochemistry: Electronic transitions in molecules, Franck-Condon principle. Electronically excited molecules- singlet and triplet states, spinorbit interaction. Quantum yield and its determination. Actinometry. Derivation of fluorescence and phosphorescence quantum yields. Quenching effect- Stern Volmer equation. Photochemical equilibrium and delayed fluorescence- E-type and P-type. Photochemical primary processes, types of photochemical reactions-photodissociation, addition and isomerization reactions with examples. | P1,P3,<br>P4,P5,<br>P10 | PQ,PT |

### **SEMESTER - III**

# **PAPER -I:** Organic reaction mechanisms, pericyclic reactions and photochemistry

| Course: M.Sc.,<br>(ORGANIC<br>CHEMISTRY) | Year/Semester: 2-1                   | Faculty Name: R.Anuradha                           |
|--|--------------------------------------|--|
| Subject                                  | PAPER -I: ORGANIO<br>REACTIONS AND P | C REACTION MECHANISMS, PERICYCLIC<br>HOTOCHEMISTRY |

| Units                  | <ul> <li>1.Radical substitution reaction</li> <li>2.Elimination reactions</li> <li>3. Addition reactions <ul> <li>a. Addition to carbon-carbon multiple bonds</li> <li>b. Addition to carbon-hetero atom multiple bonds</li> </ul> </li> <li>4. Pericyclic reactions</li> <li>5. Organic Photochemistry</li> </ul>  |   |   |   |   |  |
|------------------------|---|---|---|---|---|--|
| Learning<br>Objectives | <ul> <li>Acquire the knowledge of reactions and mechanisms of radical Substitution.</li> <li>Understand reactions and mechanisms of Elimination reactions and their stereo chemistry.</li> <li>Apply the knowledge and understanding of Addition reactions to carbon- carbon, carbon- hetero atom multiple bonds.</li> <li>Acquire the knowledge of reactions and mechanism Pericyclic reactions and their classification.</li> <li>Understand the concept of photochemistry of carbonyl compounds, unsaturated systems and aromatic</li> </ul> |   |   |   |   |  |
| Units                  | compounds U1 U2 U3 U4 U5  |   |   |   |   |  |
| Total Hours: 60        | 11 11 13 12 13  |   |   |   |   |  |
| Internal<br>Evaluation | 4   | 4 | 4 | 4 | 4 |  |

**Study Material (Handouts):** 

 $\frac{https://edscl.in/pluginfile.php/2823/mod\_resource/content/1/Teachers}{\% 20 Notes.pdf}$ 

### **Reference Books:**

- 1) Advanced Organic Chemistry: Reactions Mechanisms and Structure by Jerry March, Mc.Graw Hill and Kogakush.
- 2) Molecular reactions and Photochemistry by Charles Dupey and O. Chapman, Prentic Hall.
- 3) Pericyclic reactions by S.N. Mukharji, Mcmilan.
- 4) Mechanisms and Theory in Organic Chemistry by T.H. Lowery and K.S. Rich gardson.
- 5) The modern structural theory in Organic Chemistry by L. N. Ferguson, Pretice Hall

#### YouTube Links:

https://www.youtube.com/watch?v=Mjck01ao9Mw&list=PLj\_Alq7xw30k L1S84P\_SMO2wSfkTeN6n

### **Power Point Presentations:**

https://www.powershow.com/view0/7140c0-

ZjY3Z/photochemistry\_ppt\_powerpoint\_ppt\_presentation

### Model Question paper:

https://www.andhrauniversity.edu.in/student-corner/ug-and-pg-syllabus.html

|      | Unit - Wise Plan Pedagogical   | Evaluatio         | 11                     |
|------|--|-------------------|------------------------|
| UNIT | DESCRIPTION  | PEDAGOGY          | INTERNAL<br>EVALUATION |
| I    | Reactivity for aliphatic substrates, reactivity at Bridgehead, Reactivity in aromatic substrates, neighbouring group assistance in free radical reactions, reactivity in the attacking radical, effect of solvent on reactivity, halogenation at an alkyl carbon and allylic carbon, hydroxylation at aromatic carbon by means of Fenton's reagent, formation of cyclic ethers with Pb (OAC)4, Hunsdiecker reaction, Kolbe reaction, Reed reaction and Sandmayer reaction.   | P1,P3,<br>P5, P10 | P10,PT                 |
| п    | Elimination reactions:  Mechanisms of E2, El, and E1CB, factors-effects of substrate, attacking base, leaving group and medium. Stereochemistry of eliminations in acyclic and cyclic systems. Saytzeff elimination, Hoffman elimination and pyrolytic elimination.  | P1,P3,<br>P5, P10 | P10,PT                 |
| Ш    | Addition reactions: Addition to carbon-carbon multiple bonds- Addition reactions involving electrophiles, nucleophiles and free radicals, cyclic mechanisms. Stereochemistry and reactivity. Hydrogenation of double and triple bonds, Birch reduction, Hydroboration, Michael reaction, Prins reaction. Addition of oxygen and N2O4.  Addition to carbon-hetero atom multiple bonds: Mechanism and reactivity. Reductions of carbonyl compounds, carboxylic acids, esters, nitriles. Addition of Grignard reagents, Mannich reaction, Reformatsky reaction, Tollen's reaction, Wittig reaction. | P1,P3,<br>P5, P10 | P10,PT                 |
| IV   | <b>Pericyclic reactions:</b> Molecular Orbital Symmetry, MO diagrams of ethylene, 1,3 Butadiene, 1,3,5- Hexatriene and allyl system. Woodward- Hoffman correlation diagram method, Frontier molecular orbital approach (FMO) and Perturbation molecular orbital approach (PMO) for the explanation of pericyclic reactions under thermal and photochemical conditions.  Classification of pericyclic reactions: <b>Electrocyclic Reactions:</b> Conrotatory and Dis rotatory motions. $4n \pi$ and $4n+2 \pi$ electrons systems.   | P1,P3,<br>P5, P10 | P10,PT                 |
|      | Cycloadditions: Antarafacial and Suprafacial additions. 2+2, 4+2 cycloadditions and chelotropic reactions.  Sigma tropic rearrangements-Suprafacial and  |                   |                        |

|   | Antarafacial shifts of H, Sigmatropic shift involving carbon moieties (1,3), (1,5), (3,3) and (5,5) sigmatropic rearrangements. Claisen, Cope, Oxy-cope and aza- Cope rearrangements. Ene reaction.   |                   |        |
|---|---|-------------------|--------|
| V | Photochemistry of carbonyl compounds: $n-\pi^*$ and $\pi-\pi^*$ transitions. Norrish type I and Norrish type II cleavages. Patterno - Buchi reactions , Photoreduction, Photochemistry of $\alpha$ , $\beta$ - unsaturated ketones, photochemistry of enones and cyclohexadienones . Photochemistry of unsaturated systems (Olefins): cis - trans isomerization, dimerization, and addition . Acetylenes - dimerisation. Photochemistry of 1,3butadienes, di- $\pi$ -ethane rearrangement. Photochemistry of aromatic compounds - 1,2, 1,3, and 1,4- additions. Photo-Fries rearrangement, Photo-Fries reactions of anilides. | P1,P3,<br>P5, P10 | P10,PT |

# **PAPER -II: Organic Spectroscopy**

| Course: M.Sc., (organic chemistry) | Year/Semester: 2-1  | Faculty Name: R.ANURADHA |
|------------------------------------|---------------------|--------------------------|
| Subject                            | PAPER – II: Organio | e Spectroscopy           |

| Units                  | 2.IR Spec<br>3.NMR S<br>4.MASS   | 1.UV Spectroscopy 2.IR Spectroscopy 3.NMR Spectroscopy 4.MASS Spectroscopy 5.Structural Elucidation of Organic Compounds |   |   |   |  |
|------------------------|--|--|---|---|---|--|
| Learning<br>Objectives | <ul> <li>Acquire the knowledge of UV spectra of aromatic and hetero cyclic compounds and conformations of substituted cyclohexanones.</li> <li>Understand the characteristic vibrational frequencies of various functional groups by Infrared spectroscopy.</li> <li>Apply the knowledge and understanding the principle of NMR and its applications.</li> <li>Develop interest in the areas of Mass Spectroscopic techniques and fragmentations of various functional groups.</li> <li>To acquire the knowledge on structural elucidation of organic compounds using UV, IR, NMR, Mass</li> </ul> |  |   |   |   |  |
| Units                  | spectral data.  U1 U2 U3 U4 U5   |  |   |   |   |  |
| Total Hours: 60        | 10 13 15 9   |  |   |   |   |  |
| Internal<br>Evaluation | 4  | 4  | 4 | 4 | 4 |  |

### **Study Material (Handouts):**

https://www.utdallas.edu/~scortes/ochem/OChem\_Lab1/recit\_notes/ir\_presentation.pdf

### **Reference Books:**

- 1) Spectroscopic identification of organic compounds by RM Silverstein, G C Bassler and T B Morrill
- 2) Organic Spectroscopy by William Kemp
- 3) Spectroscopic methods in Organic chemistry by DH Williams and I Fleming
- 4) Modern NMR techniques for chemistry research by Andrew B Derome
- 5) NMR in chemistry A multinuclear introduction by William Kemp
- 6) Spectroscopic identification of organic compounds by P S Kalsi
- 7) Introduction to organic spectroscopy by Pavia
- 8) Carbon-13 NMR for organic chemists by GC Levy and O L Nelson
- 9) Nuclear Magnetic Resonance Basic principles by Atta-ur-Rahman

### YouTube Links:

https://youtu.be/jjcHZuTGWXk

https://youtu.be/XFvGQbaZPr4

https://youtu.be/2vDAyBCa5NE

**Power Point Presentations:** 

https://www.sjctni.edu/Department/ch/eLecture/Mass%20Spectrometry.ppt

Model Question paper:

https://www.andhrauniversity.edu.in/student-corner/ug-and-pg-

syllabus.html

| UNIT | Description   | PEDAGOGY         | INTERNAL<br>EVALUATION |
|------|---|------------------|------------------------|
| I    | UV-SPECTROSCOPY  UV spectra of aromatic and heterocyclic compounds, $\alpha$ -diketones, $\beta$ -diketones, enediones and quinines. Applications of UV Specroscopystudy of isomerism, determination of strength of hydrogen bonding and conformations of $\alpha$ -substituted cyclohexanones. Steric effect in biphenyls.   | P1,P3,<br>P5,P10 | PQ, PT                 |
| II   | IR_SPECTROSCOPY characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols, amines, carbonyl compounds, esters, amides, carboxylic acids, anhydrides, lactones, lactums, nitriles and conjugated carbonyl compounds. Effect of hydrogen bonding and solvent on vibrational frequencies.   | P1,P3,<br>P5,P10 | P10,PT                 |
| III  | NMR SPECTROSCOPY  Nuclear spin, resonance, satuaration, shielding of magnetic nuclei, chemical shifts and its measurements, factors affecting chemical shift, chemical and magnetic equivalence of spins, spin-spin coupling, intergration, the coupling constant, types of spin-spin couplings, factors influencing coupling constants, first-order and non-first order spectra, spin system notations (ABX, AMX, ABC, A2B2 etc.). Simplification of non-first order spectra- use of higher magnetic fields, nuclear magnetic double resonance and contact shift reagents. Deuterium exchange, nuclear overhauser effect difference spectra, Study of dynamic processes by Variable temperature (VT) NMR, restricted rotation DMF, cyclohexane ring inversion. | P1,P3,<br>P5,P10 | P10,PT                 |
| IV   | MASS SPECTROSCOPY  Basic Principles, instrumentation, isotope abundance, the molecular ion, metastable ions, base peak, fragment ions, even-electron rule and   | P1,P3,<br>P5,P10 | P10, PT                |

| V | Structural elucidation of Organic compounds: Structural elucidation of Organic compounds by a combined application of the UV, IR, NMR and MASS spectral da Structural elucidation of Organic compounds by a combined application of the UV, IR, NMR and MASS spectral data.  | P1,P3,<br>P5,P10 | P10,PT |
|---|--|------------------|--------|
|   | nitrogen rule. McLafferty rearrangement ortho effect. <i>retro</i> -Diels- Alder reaction, Fragmentation processes - fragmentation associated with various functional groups (alkanes, cycloalkanes, alkenes, alkynes, aromatic hydrocarbons, alcohols, phenols, ethers, aldehydes, ketones, esters, carboxylic acids, amides, amines, alkyl chlorides and alkyl bromides. |                  |        |

### **PAPER -III: ORGANIC SYNTHESIS**

| Course: M.Sc., (Organic chemistry) | Year-Semester: 2-1  | Faculty Name: CH.Mallika  |  |
|------------------------------------|---|---|--|
| Subject                            | Paper III- ORGANI   | C SYNTHESIS   |  |
| Units                              | <ol> <li>Formation of carbon-carbon(c-c) single bonds</li> <li>Formation of carbon-carbon double bonds</li> <li>Organic polymers</li> <li>Reactions of unactivated carbon-hydrogen bonds</li> <li>Asymmetric synthesis</li> </ol> |   |  |
| <b>Learning Objectives</b>         | via enolates, ena reagents.  • Understand form pyrolytic syn elin • Apply the knowl introduction of opolymers, proper • To understand the unactivated C-H applications.   | edge and understanding the organic rties and their classification. The concept of reactions of bonds and their synthetic in the areas of Asymmetric |  |

| Units                  | U1 | U2 | U3 | U4 | U5 |
|------------------------|----|----|----|----|----|
| Total Hours: 60        | 12 | 13 | 12 | 10 | 13 |
| Internal<br>Evaluation | 4  | 4  | 4  | 4  | 4  |

### **Study Material (Handouts):**

https://new.bhu.ac.in/Content/Syllabus/Syllabus\_3006312820200414035642.pdf

https://profiles.uonbi.ac.ke/andakala/files/sch\_302\_asymmetric\_synthesis.pdf

### **Reference Books:**

- 1. Some Modem Methods of Organic Synthesis W. Carothers, Third Edition, Cambridge University Press, Cambridge, 1988.
- 2. Modern Synthetic Reactions, Herbert O. House, Second Edition, W.A. BenzamineInc. Menio Park, California, 1972.
- 3. Principle of Organic Synthesis- R.O.C. Norman and J. M. Coxon.(ELBS)
- 4. Advanced organic chemistry part A & B; Fourth edition; Francis A Cary and Richard J. Sundberg; Kluwer Academic/Plenum Publisher New York, 2000.
- 5. Organic chemistry Jonathan Clayden, Nick Geeves, Stuart Warren, 2nd Edition, 2012, Oxford University Press.
- 6. Stereochemistry of organic compounds Principles & Applications by D Nasipuri.
- 7. Stereochemistry of Carbon compounds by Ernest L Eliel & Samuel H. wilen.
- 8. Stereochemistry: Conformation & Mechanism by P S Kalsi.
- 9. The third dimension in organic chemistry, by Alan Bassendale.
- 10. Stereo selectivity in organic synthesis by R S Ward.
- 11. Asymmetric synthesis by Nogradi.

|    | 12. Asymmetric organic reactions by J D Morrison and H S Moscher.   |
|----|---|
|    | 13. Principles in Asymmetric synthesis by Robert E. Gawley & JEFFREY  |
|    | AUBE.   |
| ₹1 | YouTube Links:<br>https://www.youtube.com/watch?v=fLXyKLVd6Hc   |
|    | Model Question paper: <a href="https://www.andhrauniversity.edu.in/student-corner/ug-and-pg-syllabus.html">https://www.andhrauniversity.edu.in/student-corner/ug-and-pg-syllabus.html</a> |
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| UNIT | DESCRIPTION   | PEDAGOGY         | INTERNAL<br>EVALUATION |
|------|---|------------------|------------------------|
| I    | Formation of Carbon-Carbon (C-C) single bonds:  A) Alkylations via enolate anions-1,3-diarbonyl and related compounds, direct alkylation of simple enolates, imine and hydrozone anions, enamines. The aldol reaction, umplong (dipole inversion)  B)via Organometallic reagents- organ palladium, organo nickel and organo copper reagents | P1,P3,P5,<br>P10 | PQ, PT                 |
| II   | Formation of carbon-carbon double   | P1,P3,P5,<br>P10 | PT,P10                 |

|    | bonds:<br>β- Elimination reactions, Pyrolytic <i>syn</i>  |                  |        |
|----|---|------------------|--------|
|    | eliminations, alkenes form hydrazones, 1,2-diols, sulfones, sulphoxide-sulphonate rearrangement, the Wittig and related reactions.  |                  |        |
| Ш  | Organic polymers Introduction to organic polymers, general properties and classification of polymers. Methods Of polymerization:(a) Addition polymerization-Definition, synthesis and applications, vulcanization. (b) Condensation Polymerization-Definition, synthesis and applications. Radical polymerization Ziegler-Natta polymerization (With atleast two examples in each category)   | P1,P3,P5,<br>P10 | PT,P10 |
| IV | Reactions of unactivated carbon-hydrogen bonds: Definition, mechanism and synthetic applications- The Hoffmann-Loeffler-Freytag reaction(HLF reaction)-cyclisation reactions of Nitrenes-the Barton reaction-Photolysis of organic hypohalites-hypochlorites, hypobromites and hypoiodites.   | P1,P3,P5,<br>P10 | PT     |
| V  | Synthetic applications of organobornaes: Organoboranes: Preparation of Organobornaes viz hydroboration with BH3-THF, dicylohexyl borane, disiamyl borane, theryl borane, 9-BBN and disopincamphlyel borne, functional group transformations of Organo boranes-Oxidation, protonolysis and rearrangements. Formation, of carbon-carbon-bonds viz organo boranes carbonylation, the cyanoborate process and reaction of alkenyl boranes and trialkenyl borates. | P1,P3,P5,<br>P10 | PQ,PT  |

### **PAPER -IV: Chemistry of Natural Products**

| PAPER -1v: Chemistry of Natural Products |  |   |  |  |  |
|--|--|---|--|--|--|
| Course: Msc., (organic chemistry)        | Year/Semester: 2-1   | Faculty Name: CH. MALLIKA   |  |  |  |
| Subject                                  | Paper IV – Chemis  | stry of Natural Products  |  |  |  |
| Units                                    | 1.Antibiotics 2.Terpenes 3.Alkaloids 4.Natural Flavanoi 5.Natural pigment  |   |  |  |  |
| Learning<br>Objectives                   | <ul> <li>elucidation,</li> <li>stereochemistry</li> <li>of selected antib</li> <li>Understand isol</li> <li>stereochemistry</li> <li>and biological p</li> <li>Apply the know</li> </ul> | ation, structural elucidation, , synthesis properties of selected terpenes eledge and understanding isolation, lation, stereochemistry, synthesis and |  |  |  |

|                        | <ul> <li>alkaloids</li> <li>Develop interest in the areas of isolation, structural elucidation, stereochemistry, synthesis and biological properties of Flavonoids</li> <li>Understand isolation, structural elucidation, stereochemistry, synthesis and biological properties of natural pigments</li> </ul> |    |    |    |    |
|------------------------|---|----|----|----|----|
| Units                  | U1  | U2 | U3 | U4 | U5 |
| Total Hours: 60        | 12 11 12 13 12  |    |    |    |    |
| Internal<br>Evaluation | 4   | 4  | 4  | 4  | 4  |

### **Study Material (Handouts):**

 $\frac{https://annamalaiuniversity.ac.in/studport/download/engg/pharm/resources/pharmd_3Y_3.5\_medicinal\%20Chemistry.pdf$ 

### **Reference Material:**

- 1. Organic Chemistry, Volume 2, Stereochemistry and chemistry of natural products, I.L. Finar, 5th Edition. ELBS.
- 2. Chemical A spects of Biosynthesis, John Mann, Oxford University Press, Oxford,1996
- 3. Chemistiy of Natural Products. A Unified Approach, N.R. Krishnaswamy, Universe.Press (India) Ltd., Orient Longman Limited, Hyderabad, 1999.
- 4. Chemistry of natural products, S. V. Bhat, Narosa Publishing House, 6th reprint 2010.

### You tube Links:

https://www.youtube.com/watch?v=K1mD55y4Yhg Model Question paper:

https://www.andhrauniversity.edu.in/student-corner/ug-and-pgsyllabus.html

| UNIT | DESCRIPTION   | PEDAGOGY    | INTERNAL<br>EVALUATION |
|------|---|-------------|------------------------|
| I    | Antibiotics-Isolation, structure, elucidation, stereochemistry, synthesis and biological properties of PencillinG, Cephalosphorin-C, streptomycin, chloramphenicol and tetracyclins | P1,P3,P4,P5 | PT,P10                 |
| II   | <b>TERPENES-</b> Isolation, structure elucidation, stereochemistry, synthesis and biological properties of Terpenes: Forskolin, taxol and β-amyrin                                  | P1,P3,P4,P5 | PQ,PT                  |
| III  | <b>Alkaloids-</b> Isolation, structure elucidation, stereochemistry, synthesis, and biological properties of Alkaloids: Morphine, reserpine and vincristine                         | P1,P3,P4,P5 | PT,P10                 |
| IV   | Natural flavonoids: Natural Flavonoids, Apigenin, flavanones, Hesperetin, Isoflavones ,Genistein, Flavonol quercetin ,xanthone- Euxanthone.   | P1,P3,P4,P5 | PQ,PT                  |
| V    | Natural pigments - Introduction structure elucidation and synthesis of quinones- Polyporic acid. Chlorophyll and haemin.  | P1,P3,P4,P5 | PQ,PT                  |

### SEMESTER – IV

PAPER -II: Modern synthetic methodology

| THE EXT II. Widdelin Symmetre interioring |   |                              |                           |                        |          |
|---|---|------------------------------|---------------------------|------------------------|----------|
| Course: M.Sc.,<br>(Organic chemistry)     | Year/Semester:2-2 Faculty Name: R:ANURADHA  |                              |                           |                        |          |
| Subject                                   | PAPE  | R- III: Modern               | Synthetic Me<br>Chemistry | thodology in O         | rganic   |
| Units                                     | 1.Modern Synthetic Methods 2.Multi component Reactions and Metathesis 3.Oxidation 4.Reduction 5.Newer methods in organic synthesis  |                              |                           |                        |          |
| Learning<br>Objectives                    | <ul> <li>Acquire the knowledge of various modern synthetic methods.</li> <li>Understand multicomponent reactions and meta thesis</li> <li>Apply the knowledge and understanding of metal and non metal based oxidations</li> <li>To understand the concept of Reduction - homogeneous and heterogeneous catalytic hydrogenation.</li> </ul> |                              |                           |                        |          |
|   |   | op interest in als and phase | · ·                       | reen chemistr<br>lysts | ry, nano |
| Units                                     | U1  | U2                           | U3                        | U4                     | U5       |
| Total Hours: 60                           | 10 10 15 15 10  |                              |                           |                        |          |
| Internal<br>Evaluation                    | 4   | 4                            | 4                         | 4                      | 4        |

### **Study Material (Handouts):**

https://www.epa.gov/greenchemistry/basics-green-chemistry

#### **Reference Books:**

- 1. Some Modern Methods of Organic Synthesis W. Carothers, Third Edition, Cambridge
- 2. University Press, Cambridge, 1988.
- 3. F. A. Cary and R. I. Sundberg, Advanced Organic Chemistry, Part A and B, 5th Edition, Springer, 2009.
- 4. M. B. Smith, Organic Synthesis, 2nd Edition, 2005
- 5. J. Tsuji, Palladium Reagents and Catalysts, New Perspectives for the 21st Century, John Wiley & Sons, 2003.
- 6. 5. I. Ojima, Catalytic Asymmetric Synthesis, 2nd edition, Wiley–VCH, New York, 2000.
- 7. J. Clayden, N. Greeves, S. Warren and P. Wothers, Organic Chemistry, Oxford University Press, 2001.
- 8. R. Noyori, Asymmetric Catalysis in Organic Synthesis, John Wiley & Sons, 1994.
- 9. L. Kuerti and B. Czako, Strategic Applications of named Reactions in Organic Synthesis Elsevier Academic Press, 2005
- 10. Green chemistry, Theory and Practical, Paul T.Anastas and John C.Warner.
- 11. New trends in green chemistry By V.K.Ahulwalia and M.Kidwai.

YouTube Links:

https://youtu.be/Zas\_JlccBNQ

https://youtu.be/PfQiyHZydtk

**Power Point Presentations:** 

https://www.slideshare.net/Krishanyadav28/synthesis-of-nanomaterials

**Model Question paper:** 

https://www.andhrauniversity.edu.in/student-corner/ug-and-pg-syllabus.html

| UNIT | DESCRIPTION   | PEDAGOGY         | INTERNAL<br>EVALUATION |
|------|---|------------------|------------------------|
| I    | Modern Synthetic Methods:  Baylis-Hillman reaction, Henry reaction, Nef reaction, Kulinkovich reaction, Ritter reaction, Sakurai reaction, Tishchenko reaction and Ugi reaction. Brook rearrangement; Tebbe olefination.  Metal mediated C-C and C-X coupling reactions: Heck, Stille, Suzuki, Negishi and Sonogashira, Nozaki-Hiyama, Buchwald-Hartwig, Ullmann coupling reaction.   | P1,P3,<br>P5,P10 | P10,PT                 |
| Ш    | Multi component Reactions: Passerini reaction, Biginelli reaction, Hantzsch reaction and Mannich reaction.  Metathesis: Grubb's 1st generation and 2nd generation catalyst, Olefin Cross coupling Metathesis (OCM), Ring Closing Metathesis(RCM), Ring Opening Metathesis (ROM) and applications.   | P1,P3,<br>P5,P10 | P10,PT                 |
| III  | Oxidation: Metal based and non-metal based oxidations of (a) alcohols to carbonyls (Chromium, Manganese, aluminium, silver, ruthenium, DMSO, hypervalent iodine and TEMPO based reagents). (b) phenols (Fremy's salt, silver carbonate) (c) alkenes to epoxides (peroxides/per acids based), Sharpless asymmetric epoxidation, Jacobsen epoxidation, Shi epoxidation.(d) alkenes to diols (Manganese, Osmium based), Sharpless asymmetric dihydroxylation, Prevost reaction and Woodward modification, (e) alkenes to carbonyls with bond cleavage (Manganese, Osmium, Ruthenium and lead based, ozonolysis) (f) alkenes to alcohols/carbonyls without bond cleavage (hydroboration-oxidation, Wacker oxidation, selenium, chromium based allylic oxidation) (g) ketones to ester/lactones (Baeyer-Villiger). | P1,P3,<br>P5,P10 | P10,PT                 |
| IV   | Reduction:  (a)Catalytic hydrogenation (Heterogeneous: Palladium/ Platinum/ Rhodium/ Nickel etc; Homogeneous: Wilkinson).  Noyori asymmetric hydrogenation. (b) Metal based   | P1,P3,<br>P5,P10 | P10,PT                 |

|   | reductions using Li/Na/Ca in liquid ammonia, Sodium, Magnesium, Zinc, Titanium and Samarium (Birch, Pinacol formation, McMurry, Acyloin formation, dehalgenation and deoxygenations) (c) Hydride transfer reagents-NaBH4 triacetoxyborohydride, L- selectride, K-selectride, Luche reduction; LiAlH4, DIBAL-H, and Red-Al. |                  |        |
|---|--|------------------|--------|
|   | Newer methods in organic synthesis:  | P1,P3,<br>P5,P10 | P10,PT |
|   | Green Chemistry: Introduction, principles, atom economy and scope (illustrate with two examples)  Microwave induced reactions: Principle conditions, advantages over conventional heating methods-applications   |                  |        |
| V | Ionic liquids: Introduction and applications in organic synthesis (illustrate with two examples).  |                  |        |
|   | Nanomaterials: Introduction, methods of preparation, applications in organic synthesis   |                  |        |
|   | Phase-transfer catalysis: solid-solid, solid-liquid systems-mechanism of catalytic action, type of catalysts, application in few important reactions   |                  |        |

# PAPER -II: Organic Spectroscopy-II

| Course: M.SC., (organic chemistry) | Year/Semester: 2-2 | Faculty Name: R.ANURADHA |
|------------------------------------|--------------------|--------------------------|
| Subject                            | PAPER II: ORGAN    | NIC SPECTROSCOPY- II     |

| Units                  | <ul> <li>1.13C NMR Spectroscopy</li> <li>2.Heteronuclear NMR Spectroscopy &amp;ESR spectroscopy</li> <li>3.NMR Instrumentation, 2D NMR Techniques</li> <li>4.Optical Rotatory Dispersion &amp; CD Spectroscopy</li> <li>5.Structural Determination of natural products by spectral methods</li> </ul>   |   |   |   |   |  |
|------------------------|---|---|---|---|---|--|
| Learning<br>Objectives | <ul> <li>Acquire the knowledge of 13C NMR spectroscopy</li> <li>Understand Heteronuclear coupling and ESR spectroscopy.</li> <li>Apply the knowledge and understanding of NMR instrumentation and 2D NMR techniques.</li> <li>Develop interest in the ORD and CD spectroscopy</li> <li>To gain knowledge on structural determination of natural products by spectroscopy</li> </ul> |   |   |   |   |  |
| Units                  | U1 U2 U3 U4 U5  |   |   |   |   |  |
| Total Hours:<br>60     | 12 12 12 12   |   |   |   |   |  |
| Internal<br>Evaluation | 4   | 4 | 4 | 4 | 4 |  |

### **Reference Books:**

- Spectroscopic Methods in Organic Chemistry. Forth Edition D.M.
   Williams and I. Fleming Tata McGraw Hill, New Delhi, 1990.
   For all spectral methods except ORD and CD and ESR.
- 2. Organic Spectroscopy, Second Edition, W.Kemp, ELBS Macmillan, 1987 for ORD and CD and ESR.
- 3. Applications of absorption spectroscopy of Organic Compounds J.R.Dyer, Prentice Hall of India, New Delhi, 1984.
- 4. Spectrometric identification of Organic Compounds, Fourth Edition, R.M. Silverstein; G.C.Vasslellr and T.C. Merill, Johne Willey, Singapore, 1981.
- 5. For ORD and CD "Applications of Optical rotation and Circular Dichroism", G.C. Barret,
- 6. "Elucidation of Organic structures by Physical and Chemical Methods" Part I (Eds) K.W. Bentley and G.W.Rirty John Wiley, 1972, Chapter VIII (only those aspects mentioned in the syllabus).

### YouTube Links:

https://youtu.be/eOKeVKjZ6Dk

https://youtu.be/q72mVbU7orE

### **Power Point Presentations:**

https://slideplayer.com/slide/15722339/

### **Model papers:**

https://www.andhrauniversity.edu.in/student-corner/ug-and-pg-syllabus.html

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| UNIT | DESCRIPTION  | PEDAGOGY         | INTERNAL<br>EVALUATION |
|------|--|------------------|------------------------|
| I    | 13C NMR spectroscopy: Introduction, 13C-chemical shifts, factors affecting the chemical shifts, chemical shifts of organic compounds. Calculation of chemical shifts of alkanes, alkenes and aromatic compounds. Types of 13C NMR spectra: Proton-coupled, proton-decoupled and OFF-resonance decoupled (ORD) spectra, DEPT. 13C-NMR solvents. | P1,P3,P5,<br>P10 | PT,P10                 |
| II   | Heteronuclear NMR spectroscopy & Electron Spin Resonance Spectroscopy (ESR): Heteronuclear couplings: 13C1H, 13C-D, 13C19F, 13C31P.1H-D, 1H19F, 1H31P, 1H15N ESR Spectroscopy: Principles, hyperfine splitting.  | P1,P3,P5,<br>P10 | PQ,P10                 |
| III  |  | P1,P3,P5,        | PT,PQ                  |

|    | NMR Instrumentation, 2D-NMR techniques NMR Instrumentation: Types of NMR Spectrometers-Continuous Wave (CW)-NMR, Fourier Transform (FT)-NMR, NMR solvents, sample preparation 2D-NMR techniques: Principles of 2D NMR, Correlation spectroscopy (COSY) HOMO COSY (1H-1H COSY), Hetero COSY (1H, 13C COSY, HMQC), long range 1H,13C COSY (HMBC), NOESY and 2D-INADEQUATE experiments and their applications             | P10              |        |
|----|--|------------------|--------|
| IV | Optical Rotatory Dispersion (ORD) and CD Spectroscopy: Optical rotation, circular birefringence, and circular dichroism and Cotton effect. Plain curves and anomalous curves. Empirical and semiempirical rules-The axial haloketone rule, the octant rule, Application of the rules to the study of absolute configuration and conformations of organic molecules   | P1,P3,P5,<br>P10 | P10,PT |
| V  | Structure determination of natural products by spectral methods: structure elucidation-Spectroscopic techniques IR, UV, 1H-NMR, 13C-NMR, COSY, HETEROCOSY, and MS- natural products- Examples, flavonesApigenin, flavanones- Hesperetin, isoflavones-Genistein, coumarins-7- hydroxycoumarin, alkaloids-morphine, quinine, terpenoids-(-) -Menthol, Steroids-stigmasterol, Glycosides-salicin (Alcoholic β-glucoside). | P1,P3,P5,<br>P10 | P10,PT |

# PAPER -III: Designing organic synthesis and synthetic applications of organo-boranes and silanes

| Course: M.Sc., (Organic chemistry) Subject | Year/Semester: 2-2 Faculty Name: CH.Mallika  Paper IV: DESIGNING ORGANIC SYNTHESIS AND SYNTHETIC APPLICATIONS OF ORGANO- BORANES  |
|--|---|
|  | AND -SILANES  |
| Units                                      | <ol> <li>1.Disconnection approach –Principles</li> <li>2. Synthetic Strategies-One group disconnections</li> <li>3. Synthetic Strategies-Two group disconnections</li> <li>4. Organoboranes</li> <li>5. Organo Silanes</li> </ol> |

| Learning Objectives         | <ul> <li>diapri</li> <li>U</li> <li>oi</li> <li>A</li> <li>oi</li> <li>A</li> <li>gi</li> <li>D</li> <li>oi</li> <li>sy</li> <li>Un</li> </ul> | <ul> <li>Acquire the knowledge of the disconnection approach and its principles.</li> <li>Understand the synthetic strategies for one group disconnection</li> <li>Apply the knowledge and understanding of disconnection</li> <li>Approach, synthetic strategies in two group disconnection</li> <li>Develop interest in the areas of the organo boranes preparations and their synthetic applications.</li> <li>Understand the preparations and synthetic applications of organosilanes</li> </ul> |    |    |    |
|-----------------------------|--|--|----|----|----|
| Units                       | U1 U2 U3 U4 U5   |  |    |    |    |
| Total Hours: 60             | 14   | 10   | 11 | 13 | 12 |
| Internal Evaluation:<br>20M | 4 4 4 4  |  |    |    |    |

### **Study Material (Handouts):**

https://www.massey.ac.nz/~gjrowlan/chem312/tutorial.pdf

### Reference Books:

- 1. Organic syntheses via boranes / Herbert C. Brown; with techniques by Gary.W. Kramer, Alan B. Levy, M. Mark Midland. New York: Wiley, 1975
- 2. Some Modern Methods of Organic Synthesis W. Carothers, Third Edition, Cambridge University Press, Cambridge, 1988.
- 3. Organic Synthesis: The disconnection approach, S. Warrant John Wiley & sons, New York, 1984.
- 4. 4. Modern Synthetic Reactions, Herbert O. House, Second Edition,
- 5. W.A. Benzamine, Inc. Menio Park, California, 1972.
- 6. Principle of Organic Synthesis-R.O.C. Norman and J. M. Coxon.(ELBS)
- 7. Organic Synthesis: Special techniques. V.K.Ahulwalia and Renu Aggarwal.
- 8. Organic Synthesis by C Willis and M Willis
- 9. Problems on organic synthesis by Stuart Warren

### YouTube Links:

https://www.youtube.com/watch?v=0XJEgJ8OD28

https://www.youtube.com/watch?v=KsMXXgbhVkk

### **Model Question paper:**

https://www.andhrauniversity.edu.in/student-corner/ug-and-pg-syllabus.html

| UNIT | DESCRIPTION   | PEDAGOGY | INTERNAL<br>EVALUATION |
|------|---|----------|------------------------|
| I    | Disconnection approach —Principles  Introduction, Terminology: Retrosynthesis, Target Molecule (TM), synthon, synthetic equivalent, functional group interconversion (FGI). Linear and convergent synthesis. Criteria for selection oftarget. Order of events in retrosynthesis with reference to Salbutamol, Proparcaine and Dopamine. Chemoselectivity, Regioselectivity, reversal of polarity and cyclizations. Protecting groups- Principles of protection of alcohols, amine, carbonyl and carboxyl groups | P1,P3,P5 | PT,P10                 |
| II   | Synthetic Strategies-One group disconnections  Introduction to one group disconnections: C-C disconnection-alcohols and carbonyl compounds; C-X disconnections- alcohols and carbonyl compounds and sulphides two group C-C and C-X Disconnections.   | P1,P3,P5 | PQ,P10                 |
| III  | Synthetic Strategies-Two group disconnections  Introduction to Two group C-C disconnections; Diels-Alder reaction, 1,5-difunctionalised compounds, Michael addition and Robinson annulation. Two group C-X disconnections; 1, 1-difunctionalised, 1, 2-difunctionalised and 1, 3- difunctionalised compounds. Control in carbonyl condensations, explanation with examples oxanamide and mevalonic acid.  | P1,P3,P5 | PQ,P10                 |
| IV   | Organoboranes  Hydroboration- Preparation of Organoboranes. Reagents —dicylohexyl borane, disiamyl borane, thexyl borane, 9-BBN and mono-, di- isopinocampheyl borane. Functional group transformations of Organo boranes-Oxidation, protonolysis   | P1,P3,P5 | PT,PQ                  |

|   | and rearrangements. Formation of carbon-<br>carbon-bonds viz organo boranes-<br>carbonylation, cyanoboration  |                  |       |
|---|---|------------------|-------|
| V | Organo Silanes  Preparation and synthetic applications of trimethylsilyl chloride, dimethyltutylsilyl chloride, trimethylsilyl cyanide, trimethylsilyl iodide and trimethylsilyl triflate. Protection of functional groups- Trimethylsilyl ethers, Silyl enol ethers. Synthetic applications of $\alpha$ -silyl carbanions, $\beta$ -silyl carbonium ions. Peterson's olefination | P1,P3,P5,<br>P10 | P4,PT |

### PAPER -IV: DRUG DESIGN AND DRUG CHEMISTRY

| Course: Msc., (organic chemistry) | Year/Semester:   | 2-2 Fa | culty Name: CH | . MALLIKA |    |
|-----------------------------------|--|--------|----------------|-----------|----|
| Subject                           | Paper IV – DRUG DESIGN AND DRUG CHEMISTRY  |        |                |           |    |
| Units                             | <ol> <li>Basic consideration of drugs</li> <li>Antineoplastic Agent</li> <li>Cardiovascular Drugs</li> <li>Oral Hypoglycemic Drugs</li> <li>Local Anti-infective Drugs &amp; Antiviral drugs</li> </ol>  |        |                |           |    |
| Learning objectives               | <ul> <li>Acquire the knowledge of drugs, their classification, drug metabolism and drug development, Structure Activity Relationship in drugs</li> <li>Understand drugs, their classification, drug metabolism of antineoplastic drugs</li> <li>Understand drugs, their classification, drug metabolism of cardiovascular drugs</li> <li>Acquire the knowledge of oral hypoglycemic drugs.</li> <li>Apply the knowledge and understanding of local antinifective and antiviral drugs.</li> </ul> |        |                |           |    |
| Units                             | U1 U2 U3 U4 U5   |        |                |           |    |
| Total Hours : 60                  | 12   | 11     | 12             | 11        | 14 |
| Internal<br>Evaluation            | 4  | 4      | 4              | 4         | 4  |

### **Study Material (Handouts):**

https://baranlab.org/wp-content/uploads/2018/10/Final-Slides-1.pdf

#### Reference books:

- 1. Text book of medicinal chemistry, volume I & II, Third Edition by V alagarsamy, CBS- publishers
- 2. Introduction to medicinal chemistry, A. Gringuage Wiley VCH
- 3. Wilson and Gisvolds text book of organic medicinal and pharmaceuiticalchemistry, Ed Robert F Dorge
- 4. An introduction to Drug Design., S. S Pandeyeaand J.R Dimmock, New age international
- 5. Burgers Medicicnal chemistry and Drug discovery, Vol-1(chapter -9 and chap -14)Ed M E Wollff, john Wiley
- 6. Good man Gillman Pharamacological Basis of Therapeutics, McGraw-Hill
- 7. The Organic chemistry of drug design and drug action, R. B Silverman Acedamic Press
- 8. Strategies of organic drug synthesis and design, D. Lednieer. John Wiley

### YouTube Links:

https://www.youtube.com/watch?v=LWDQyaKVols

https://www.youtube.com/watch?v=0tLYC89tRPc

### Model Question paper:

https://www.andhrauniversity.edu.in/student-corner/ug-and-pg-syllabus.html

| UNIT | DESCRIPTION   | PEDAGOGY        | INTERNAL<br>EVALUATION |
|------|---|-----------------|------------------------|
| Ι    | Basic consideration of drugs: General Classification, nomenclature, drug metabolism. Development of drugs: Procedure followed in drug design, concepts of lead compound lead modification, concept of prodrugs, Structure Activity Relationship (SAR)- factors affecting bioactivity-resonance, inductive effect, isosterism, bioisosterism, spatial considerations, Qunatitative Structure Activity Relationships (QSAR)-Concepts of drug receptors. Elementary treatment of drug receptor interactions. Physico-chemical parameters: lipophilicity, partition coefficient, electronic ionization constants, steric, Shelton and surface activity parameters and redox potentials. | P1,P2,P3,<br>P5 | PQ,P10                 |
| II   | Antineoplastic Agents:  Introduction, classification-alkylating agents- mechanism and mode of action, nitrogen mustards- synthesis, properties, uses and dosage - Chlorambucil, cyclophosphamide and melphalan. Antimetabolites- synthesis, properties, uses and dosage-pyrimidine analogues-5-flurouracil, purine analogues-6-mercaptopurine, folic acid analogues- Methotrexate. Antibiotics-structure, properties and dosage-Doxorubicin, Mitomycin  | P1,P2,P3,<br>P5 | PT, P10                |
| III  | Cardiovascular Drugs:  Introduction, cardiovascular diseases, drug inhibitors of peripheral sympathetic function, central intervention of cardiovascular output. Direct acting arteriolar dilators. Synthesis of amyl nitrate, sorbitrate, diltiazem, quinidine, verapamil, methyldopa, atenolol, oxyprenolol.  | P1,P2,P3,<br>P5 | PT, PQ                 |

| IV | Oral Hypoglycemic Drugs: Introduction, Classification, Sulphonylureas- synthesis, mode of action, properties, uses and dosage- tolbutamide, glipizide. Biguanides- synthesis, mode of action, properties, uses and dosage-Metformin. α-glucosidage inhibitors-synthesis, mode of action, properties, uses and dosage-Miglitol. Dipeptidyl Peptidase-4 (DPP-4) inhibitors-synthesis, mode of action, properties, uses and dosage-saxagliptin and sitagliptin  | P1,P2,P3,<br>P5 | PT, PQ  |
|----|--|-----------------|---------|
| V  | Local Antiinfective Drugs: Introduction and general mode of action. Synthesis of sulphonamides, ciprofloxacin, norfloxacin, dapsone, amino salicylic acid, isoniazid, fluconazole, econozole and chloroquin.  Antiviral Drugs: Introduction, classification based on mechanism of action, Nucleoside or Nucleotide Reverse Transcriptase Inhibitors (NRTIs)-Synthesis, metabolism, properties and uses and dosage-Acyclovir, Zidovudine (Anti-HIV agent). Non-Nucleoside or Nucleotide Reverse Transcriptase Inhibitors (NNRTIs)-Synthesis, metabolism, properties and uses and dosage-Nevirapine, Efavirenz. Protease Inhibitors (PIs)- Synthesis, metabolism, properties and uses and dosage-Indinavir. CCR5-Inhibitors- Synthesis, metabolism, properties and uses and dosage-Indinavir. CCR5-Inhibitors- Synthesis, metabolism, properties and uses and dosage-Maraviroc | P1,P2,P3,<br>P5 | PT, P10 |