

## NEP Syllabus: PG 2 Years Chemistry

| Semester     | Course Type                                    | Paper Code    | Course                                                                    | Credit |
|--------------|------------------------------------------------|---------------|---------------------------------------------------------------------------|--------|
| I            | DSC                                            | CHEM-DSC-101  | Organic Chemistry Theory                                                  | 4      |
|              | DSC                                            | CHEM-DSC-102  | Inorganic Chemistry Theory                                                | 4      |
|              | DSC                                            | CHEM-DSC-103  | Physical Chemistry Theory                                                 | 4      |
|              | DSC                                            | CHEM-DSC-104  | Physical Chemistry Practical                                              | 4      |
|              | DSE                                            | CHEM-DSE-105A | Molecular Spectroscopy-I                                                  | 4      |
|              |                                                | CHEM-DSE-105B | Molecular Spectroscopy-II                                                 |        |
|              |                                                | CHEM-DSE-105C | SWAYAM MOOCs Course                                                       |        |
|              | Skill based Course                             | CHEM-SEC-106  | Techniques in Organic Chemistry                                           | 4      |
| Total Credit |                                                |               |                                                                           | 24     |
| II           | DSC                                            | CHEM-DSC-201  | Organic Chemistry Theory                                                  | 4      |
|              | DSC                                            | CHEM-DSC-202  | Inorganic Chemistry Theory                                                | 4      |
|              | DSC                                            | CHEM-DSC-203  | Physical Chemistry Theory                                                 | 4      |
|              | DSC                                            | CHEM-DSC-204  | Inorganic Chemistry Practical                                             | 4      |
|              | DSE                                            | CHEM-DSE-205A | Molecular Spectroscopy-III                                                | 4      |
|              |                                                | CHEM-DSE-205B | Molecular Spectroscopy-IV                                                 |        |
|              |                                                | CHEM-DSE-205C | SWAYAM MOOCs Course                                                       |        |
|              | Skill based Course                             | CHEM-SEC-206  | Synthetic Organic Chemistry                                               | 4      |
| Total Credit |                                                |               |                                                                           | 24     |
| III          | DSC                                            | CHEM-DSC-301  | Physical Chemistry Theory                                                 | 4      |
|              | DSE                                            | CHEM-DSE-302A | Organic Chemistry Theory                                                  | 4      |
|              |                                                | CHEM-DSE-302B | Advance Organic Chemistry Theory                                          |        |
|              | DSE                                            | CHEM-DSE-303A | Inorganic Chemistry Theory                                                | 4      |
|              |                                                | CHEM-DSE-303B | Supramolecular Chemistry, Crystal Engineering and Inorganic Nanomaterials |        |
|              |                                                | CHEM-DSE-303C | SWAYAM MOOCs Course                                                       |        |
|              | Advance Research Methodology                   | CHEM-DRP-304  | Advance Research Methodology                                              | 4      |
|              | Dissertation/Research Project/Entrepreneurship | CHEM-DRP-305  | Dissertation/Research Project/Entrepreneurship                            | 8      |
| Total Credit |                                                |               |                                                                           | 24     |
| IV           | DSC                                            | CHEM-DSC-401  | Industrial and analytical chemistry                                       | 4      |
|              | DSE                                            | CHEM-DSE-402A | Physical Chemistry Theory                                                 | 4      |
|              |                                                | CHEM-DSE-402B | Advance Physical Chemistry Theory                                         |        |
|              | DSE                                            | CHEM-DSE-403A | Organic Chemistry Theory                                                  | 4      |
|              |                                                | CHEM-DSE-403B | Advance Organic Chemistry Theory                                          |        |
|              |                                                | CHEM-DSE-403C | SWAYAM MOOCs Course                                                       |        |
|              | Dissertation/Research Project/Entrepreneurship | CHEM-DRP-404  | Dissertation/Research Project/Entrepreneurship                            | 12     |
| Total Credit |                                                |               |                                                                           | 24     |

## NEP Syllabus: PG 2 Years Chemistry, Semester – I

| Semester            | Course Type        | Paper Code    | Course                          | Credit    |
|---------------------|--------------------|---------------|---------------------------------|-----------|
| I                   | DSC                | CHEM-DSC-101  | Organic Chemistry Theory        | 4         |
|                     | DSC                | CHEM-DSC-102  | Inorganic Chemistry Theory      | 4         |
|                     | DSC                | CHEM-DSC-103  | Physical Chemistry Theory       | 4         |
|                     | DSC                | CHEM-DSC-104  | Physical Chemistry Practical    | 4         |
|                     | DSE                | CHEM-DSE-105A | Molecular Spectroscopy-I        | 4         |
|                     |                    | CHEM-DSE-105B | Molecular Spectroscopy-II       |           |
|                     |                    | CHEM-DSE-105C | SWAYAM MOOCs Course             |           |
|                     | Skill based Course | CHEM-SEC-106  | Techniques in Organic Chemistry | 4         |
| <b>Total Credit</b> |                    |               |                                 | <b>24</b> |

**Paper Code: CHEM-DSC-101**

**Course Title:** Organic Chemistry Theory  
**Contact Hrs:** 4 Lectures per Week  
**Examination Duration (Hrs.):** Two Hours  
**Mode of Evaluation:**  
**Continuous Assessment (CA):** 10 Marks  
**End term Examination (ETE):** 40 Marks  
**Total Credits:** 4  
**Semester:** I  
**Subject Area:** Organic Chemistry  
**Objective:** To acquire knowledge about the structure reactivity of organic molecules and intermediates, stereochemistry and pericyclic reaction.

| Unit                       | Contents                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          | Contact Hrs |           |
|----------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------|-----------|
|                            |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | L           | T         |
| 1                          | <b>Structure Reactivity Relationship:</b> MO treatment of acyclic and cyclic conjugated systems: Huckel treatment; applications to ethylene, allyl, cyclopropenyl, butadiene, cyclobutadiene, Benzene. Graphical methods; Frost diagram. Hückel's rule and concept of aromaticity, annulenes, heteroannulenes, fullerenes(C60), alternant and non-alternant hydrocarbons, anti-aromaticity, pseudo-aromaticity, homo-aromaticity. Hammett equation and Taft equation.                                                                                                                                                                                                                                                                                                                                                                                                                             | 12          | 4         |
| 2                          | <b>Stereochemistry:</b> Nomenclature; Axial and planar chirality and helicity; Correlation of axial dissymmetry and Centrodissymmetry. Prochirality and Prostereoisomerism; Topicity of Ligands and Faces: homotopicity, enantiotopicity, diastereotopicity and nomenclature. Symmetry elements and operations, point group, symmetry number, order of Point Groups, achiral Point Groups. Molecular dissymmetry and optical activity.<br>Conformational analysis of cyclic system; mono, di and polysubstituted cyclohexanes, regiospecific and regioselective reactions, stereoselective and stereospecific reactions, base-induced and pyrolytic eliminations, solvolysis, esterification, hydrolysis, oxidation, reduction, neighbouring group participation reactions of acyclic and cyclic molecules.<br>Brief idea on fused ring system-decalin, perhydroanthracene, perhydrophenanthrene. | 12          | 4         |
| 3                          | <b>Organic Reaction Mechanism:</b> Types of Mechanism, types of Reactions, importance of product analysis, reactive intermediates and their detection, information from reaction kinetics, reaction energetics, energy profile diagrams, activation parameters, primary and secondary kinetic isotope effects, solvent effects, kinetic and thermodynamic controls, Hammond postulates, guidelines for proposing reaction mechanism. With special emphasis on substitution and Elimination reactions.                                                                                                                                                                                                                                                                                                                                                                                             | 12          | 4         |
| 4                          | <b>Pericyclic Reactions:</b> Orbital symmetry, frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene, allylic system, FMO approach, Woodward-Hoffman correlation diagram method, Aromatic transition state approach, pericyclic reactions under thermal and photochemical conditions; electrocyclic reactions-conrotatory and disrotatory motions, [4n], [4n+2] allyl systems, cyclo addition-[4n], [4n+2] systems with emphasis on [2+2] and [4+2] cyclo additions, stereochemical and substituent effects, sigmatropic rearrangements-shifts of H and carbon moieties, detailed treatment of Claisen, Cope, Sommelet-Hauser, Wittig rearrangements, Cheletropic reaction, group transfer reaction, torquoselectivity                                                                                                                                                                   | 12          | 4         |
| 5                          | <b>Reactive Intermediates:</b> Generation, structure, stability, and reactivity of carbanion, carbocations, radicals, carbenes, benzyne and nitrenes. Application of Sulfur and nitrogen Ylides in organic synthesis.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | 12          | 4         |
| <b>Total Contact Hours</b> |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | <b>60</b>   | <b>20</b> |

**Recommended Books:**

1. F.A. Carey and R.J. Sundberg, Advanced Organic Chemistry Part A and Part B, 4<sup>th</sup>Edn., Plenum Press, New York
2. E. L. Eliel, S.H. Wilen and L.N. Mander, Stereochemistry of Organic Compounds, John Wiley & Sons, New York
3. March's Advanced Organic Chemistry, 4<sup>th</sup> edition
4. D. Nasipuri, Stereochemistry of Organic Compounds, Wiley Eastern, New Delhi.
5. Organic Chemistry. Clayden, Greeves, Warren.
6. Molecular Orbitals and Organic Chemical Reactions. Ian Fleming, Wiley, 2009.
7. Hückel Molecular Orbital Theory. Keith Yates.
8. Pericyclic Reactions: A Mechanistic Study, S. M. Mukherji.
9. Pericyclic Reactions: A Mechanistic and Problem-Solving Approach. Sunil Kumar, Vinod Kumar, S.P. Singh.
10. Pericyclic Reactions. Chapman and Hall Chemistry Textbook Series.
11. The Hammett equation. C.D. Johnson.

**Paper Code: CHEM-DSC-102**

**Course Title:**Inorganic Chemistry Theory

**Contact Hrs:** 4 Lectures per Week

**Examination Duration (Hrs.):** Two Hours

**Mode of Evaluation:**

**Continuous Assessment (CA):** 10 Marks

**End term Examination (ETE):** 40 Marks

**Total Credits:** 4

**Semester:** I

**Subject Area:**Inorganic Chemistry

**Objective:** To acquire comprehensive knowledge of coordination chemistry, bonding theories, organometallic chemistry, materials chemistry, and metal–ligand equilibria in solution.

| Unit | Contents                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            | Contact Hrs |   |
|------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------|---|
|      |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | L           | T |
| 1    | <p><b>Coordination Chemistry:</b> Experimental evidence of metal–ligand orbital overlap; spin–orbit coupling constants and interelectronic coupling parameters in complex ions compared with free ions; the nephelauxetic effect; adjusted Crystal Field Theory (CFT); hole formalism; tetrahedral distortion and the Jahn–Teller effect (static and dynamic); the influence of crystal field stabilization on ionic radii, lattice energy, hydration enthalpy, and the stability of complexes (Irving–Williams order); colour and electronic spectra; kinetic aspects of crystal field stabilization, including crystal field activation energy; limitations of Crystal Field Theory; and the concepts of labile and inert complexes.</p> <p><b>Electronic Spectra of Transition Metal Complexes:</b> Microstates; Russell–Saunders term symbols; determination of the ground and excited state terms of <math>d^n</math> ions; qualitative interpretation using Orgel diagrams; selection rules for spectral transitions; d–d spectra of <math>d^n</math> ions and evaluation of crystal field parameters; the nephelauxetic series; and Molecular Orbital Theory (MOT) to explain <math>\sigma</math> (sigma) and <math>\pi</math> (pi) bonding interactions in octahedral, square planar, and tetrahedral metal complexes, including symmetry designations of ligand group orbitals (LGOs) and molecular orbitals (MOs), along with simplified molecular orbital diagrams.</p>                                                                                                                                                                                                                                                  | 12          | 4 |
| 2    | <p><b>Organometallic Chemistry:</b> Introduction to organotransition metal chemistry, including its history, the nature of metal–carbon bonding, and the definition and classification of organometallic compounds. Classification of ligands, along with the kinetic and thermodynamic stability of organometallic compounds.</p> <p>Study of compounds containing metal–carbon <math>\sigma</math> (sigma) and multiple bonds, including hapticity in metal–alkyl, allyl, aryl, carbene (Fischer and Schrock types), carbonyl, carbyne, and cyclopentadienyl complexes. Topics include their synthesis, bonding, stability, reactivity, decomposition pathways, and the various reactions of organometallic compounds. Structure and bonding in <math>\eta^2</math>-ethylenic and <math>\eta^3</math>-allylic complexes with suitable examples, as well as the structure and bonding of complexes such as <math>K[Pt(C_2H_4)Cl_3]</math>, <math>[(Ph_3P)_2Pt(Ph-C\equiv C-Ph)]</math>, and metallocycles.</p> <p><b>Fluxional Organometallic Compounds:</b> Concepts of fluxionality and dynamic equilibria in organometallic compounds, including <math>\eta^2</math>-olefin, <math>\eta^3</math>-allyl, and dienylic complexes. Agostic interactions and the experimental techniques used to study fluxional behaviour and bonding of <math>K[Pt(C_2H_4)Cl_3]</math>, <math>[(Ph_3P)_2Pt(Ph-C\equiv C-Ph)]</math> and metallocycles are also included.</p>                                                                                                                                                                                                                                                                      | 12          | 4 |
| 3    | <p><b>Materials Chemistry</b></p> <p><b>Solid-State Chemistry:</b> Theory of crystalline solids; the free electron model and its limitations; the Kronig–Penney model; band theory and band gap; molecular electronics; properties of metals, insulators, and semiconductors; intrinsic and extrinsic semiconductors; p–n junction semiconductors; superconductors; rectifiers and transistors; and point defects in crystals, including Schottky and Frenkel defects.</p> <p><b>Supramolecular Chemistry:</b> Basic concepts and principles of supramolecular chemistry; molecular recognition and host–guest interactions; anion coordination and recognition of anionic substrates; organometallic receptors and their host–guest complexes; spherical recognition; podands, podates, cryptands, cryptates, and crown ethers; molecular devices and supramolecular assemblies; supramolecular orbitals; supramolecular arrays such as ribbons, ladders, racks, braids, and grids; and the use of non-covalent interactions in designing functional materials. The syllabus also covers receptors and receptor–substrate complexes, dendrimers, polycatenanes, interlocking compounds, metal–organic frameworks (MOFs), and their applications.</p> <p><b>Nanochemistry:</b> History and development of nanoscience; definitions related to the nanoworld; Nanomaterials used in ancient India; properties of nanomaterials; typical synthetic strategies for preparing nanomaterials; modern characterization techniques, with emphasis on Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), and Atomic Force Microscopy (AFM); and applications of nanomaterials in various fields of science and</p> | 12          | 4 |

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|----------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------|-----------|
|                            | technology.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |           |           |
| 4                          | <b>Theories of Bonding:</b> Introduction to the Heitler–London theory of the hydrogen molecule and the Molecular Orbital Theory (MOT). Study of the salient features of Valence Bond Theory (VBT) and Molecular Orbital Theory (MOT), along with a comparative understanding of the two approaches. Bonding in homonuclear and heteronuclear diatomic molecules of the second period, including the construction and interpretation of molecular orbital (MO) diagrams. Bonding in triatomic molecules such as $\text{H}_3^+$ , $\text{BeH}_2$ , and $\text{H}_2\text{O}$ ; tetraatomic molecules such as $\text{BH}_3$ and $\text{NH}_3$ ; and the methane molecule ( $\text{CH}_4$ ). Study of Walsh diagrams and their applications in understanding molecular geometry. Structure prediction using the Valence Shell Electron Pair Repulsion (VSEPR) theory and hybridization model, including Bent's rule. Application of Valence Bond Theory to explain the bonding in the hydrogen ( $\text{H}_2$ ) molecule. | 12        | 4         |
| 5                          | <b>Metal–Ligand Equilibria in Solution:</b> Study of the stability of mononuclear, polynuclear, and mixed-ligand complexes in solution. Concepts of stepwise and overall formation (stability) constants, their relationships, and the trends observed in stepwise formation constants. Factors affecting the stability of metal complexes, with particular emphasis on the nature of metal ions and ligands. The influence of statistical and non-statistical factors on the stability of complexes in solution. Stability and reactivity of mixed-ligand complexes, including the chelate effect, thermodynamic considerations, and the macrocyclic and template effects. Determination of binary formation constants using spectrophotometric and pH-metric methods.                                                                                                                                                                                                                                              | 12        | 4         |
| <b>Total Contact Hours</b> |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | <b>60</b> | <b>20</b> |

**Recommended Books:**

1. Inorganic Chemistry — Housecroft & Sharpe
2. Advanced Inorganic Chemistry — Cotton & Wilkinson
3. Inorganic Electronic Spectroscopy — Lever
4. Supramolecular Chemistry — Steed & Atwood
5. Solid State Chemistry and Its Applications — Anthony R. West
6. Basic Organometallic Chemistry: Concepts, Syntheses and Applications — B. D. Gupta, A J Elias

| Paper Code: CHEM-DSC-103                                                                                                                                                                                                                                                                                                                                                                                                                                                      |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |             |           |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------|-----------|
| <b>Course Title:</b> Physical Chemistry Theory<br><b>Contact Hrs:</b> 4 Lectures per Week<br><b>Examination Duration (Hrs.):</b> Two Hours<br><b>Mode of Evaluation:</b><br><b>Continuous Assessment (CA):</b> 10 Marks<br><b>End term Examination (ETE):</b> 40 Marks<br><b>Total Credits:</b> 4<br><b>Semester:</b> I<br><b>Subject Area:</b> Quantum Mechanics, Group Theory<br><b>Objective:</b> To acquire knowledge and application of quantum theory and group theory. |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |             |           |
| Unit                                                                                                                                                                                                                                                                                                                                                                                                                                                                          | Contents                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | Contact Hrs |           |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         | L           | T         |
| 1                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | <b>Introduction to Quantum Mechanics:</b> Wave-particle duality. Uncertainty principle. Postulates of Quantum Mechanics. Schrodinger wave equation and its solution. Wavefunction and its probabilistic interpretation. Orthogonality and normalization of wavefunctions. Operator and related theorems. Linear operators. Hermitian operators. Kinetic energy operator. Eigenvalue equation. Commutation relation. Operator and observables. Non-commuting operators and uncertainty relation. Heisenberg's equation of motion. Virial theorem.                                                        | 12          | 4         |
| 2                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | <b>Free Particle and Particle-in-Box:</b> Free Particle. Particle-in-Box and energy quantization. Selection Rules. Discussion on Bohr's correspondence principle. Checking the validity of Schrodinger wave equation based on correspondence principle and Heisenberg's Uncertainty principle. Quantum Mechanical Tunnelling.                                                                                                                                                                                                                                                                           | 12          | 4         |
| 3                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | <b>Harmonic Oscillator:</b> Solution of Schrodinger equation of a Harmonic oscillator using the operator method as well as the technique for solution of differential equation. Traditional solution of the Schrödinger equation for a 1D harmonic oscillator, Recursion relation, Selection rules for Harmonic oscillator. Checking the validity of Schrodinger wave equation based on correspondence Heisenberg's Uncertainty principle.                                                                                                                                                              | 12          | 4         |
| 4                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | <b>Group Theory-I:</b> Introduction to symmetry. Symmetry elements and Symmetry operations. Definition of a Group. Point symmetry groups. Group multiplication tables. Theorems of groups. Conjugate elements and class. Symmetry Operators and their Matrix Representation. Reducible and irreducible representations. Equivalent representations. Characters of representations.                                                                                                                                                                                                                      | 12          | 4         |
| 5                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | <b>Group Theory-II:</b> Great Orthogonality Theorem- statement and interpretation. Proof of its corollaries. Character table and its construction. Number of times an irreducible representation occurs in a reducible one. The reduction of reducible representations. Notation of irreducible representations. Representations and quantum mechanics. The invariance of Hamiltonian operator under symmetry transformations. Direct product representation. Molecular vibrations. Symmetry species of the vibrational mode. Selection rules for Infra-red and Raman spectra. Crystal field splitting. | 12          | 4         |
| <b>Total Contact Hours</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                    |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         | <b>60</b>   | <b>20</b> |

**Recommended Books:**

1. Quantum Chemistry by Donald A McQuarrie
2. Quantum Mechanics second edition, by V. Devanathan
3. Quantum Chemistry fifth edition by Ira N. Levine
4. Atkins'Physical Chemistry tenth edition by Peter Atkins and Julio de Paula
5. Chemical Applications of Group Theory third edition by F. Albert Cotton
6. Group Theory in chemistry Bonding and Molecular spectroscopy by Asok K Mukherjee and Bankim Chandra Ghosh
7. Symmetry and Group Theory in Chemistry by R Ameta
8. A text book of Physical Chemistry, Quantum chemistry and Molecular Spectroscopy, volume 4 by K.L Kapoor
9. Introduction to Quantum Mechanics — D. J. Griffiths & D. F. Schroeter
10. Quantum Mechanics: Concepts and Applications — NouredineZettili
11. Principles of Quantum Mechanics — R. Shankar
12. Introductory Quantum Mechanics — Richard L. Liboff
13. Modern Quantum Mechanics — J. J. Sakurai & Jim Napolitano
14. Quantum Mechanics, Vol. 1 & 2 — Cohen-Tannoudji, Diu & Laloë

**Paper Code: CHEM-DSC-104**

**Course Title:** Physical Chemistry Practical

**Contact Hrs:** 8 Contact Hours per Week

**Examination Duration (Hrs.):** Five Hours

**Mode of Evaluation:**

**Continuous Assessment (CA):** 10 Marks

**End term Examination (ETE):** 40 Marks

**Total Credits:** 4

**Semester:** I

**Subject Area:** Physical Chemistry Laboratory Work

**Objective:** To acquire practical knowledge about pH, potentiometric titration, kinetic study and colorimetric study.

| Unit | Contents                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |
|------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 1    | <ol style="list-style-type: none"><li>1. Studies on the kinetics of iodination of acetone (iodine effect/acetone effect/acid effect).</li><li>2. To determine the formal potential of FeIII/FeII couple by potentiometry.</li><li>3. To determine the rate constant and salt effect on the rate constant of decomposition of <math>K_2S_2O_8</math> by KI.</li><li>4. Studies on alkaline hydrolysis of ethylacetate conductometrically.</li><li>5. To study the kinetics of alkaline hydrolysis of crystal violet by spectrophotometry</li><li>6. Estimation of strong and a weak acid in a given mixture by pH metrically.</li><li>7. Determination of Hydrolytic Constant (<math>K_h</math>) of Ammonium Chloride solution pH-metrically.</li><li>8. Determination of <math>pK_a</math> values of phosphoric acid of any dibasic acid pH- metrically at laboratory temperature.</li><li>9. Potentiometric titration of Zn(II) solution by Potassium Ferrocyanide solution and also determination of the composition of Zn(II) Ferrocyanide complex.</li><li>10. Determination of Eo of <math>Ag^+/Ag</math> electrode and solubility product of AgCl.</li><li>11. Estimation of Cl<sup>-</sup>, Br<sup>-</sup> and I<sup>-</sup> in a mixture potentiometrically.</li><li>12. To Determine the composition and stability constant of Fe(III)-Salicylic acid complex colorimetrically.</li></ol> |

**Recommended Books:**

1. Physical Chemistry Practical by Saroj Kr Maity, Naba Kr. Ghosh
2. An Advanced Course in Practical Chemistry by Ghosha Mahapatra Nad

| Paper Code: CHEM-DSE-105A                                                                                                                                                                                                                                                                                                                                                                                                                                                     |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |             |           |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------|-----------|
| <b>Course Title:</b> Molecular Spectroscopy – I<br><b>Contact Hrs:</b> 4 Lectures per Week<br><b>Examination Duration (Hrs.):</b> Two Hours<br><b>Mode of Evaluation:</b><br><b>Continuous Assessment (CA):</b> 10 Marks<br><b>End term Examination (ETE):</b> 40 Marks<br><b>Total Credits:</b> 4<br><b>Semester:</b> I<br><b>Subject Area:</b> Molecular Spectroscopy<br><b>Objective:</b> To acquire knowledge about the theory and application of molecular spectroscopy. |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |             |           |
| Unit                                                                                                                                                                                                                                                                                                                                                                                                                                                                          | Contents                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | Contact Hrs |           |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | L           | T         |
| 1                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | <b>Introduction and Spectroscopic Transition:</b> Theory of Electromagnetic Radiation. Interaction between Matter and Electromagnetic Radiation– Semi classical treatment, Time-dependent perturbation Theory. Fermi golden rule, Transition probabilities and rates, Lambert-Beer's Law. Spectral shapes, Decoupling of the nuclear and electronic motions in a molecule: Born-Oppenheimer approximation.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | 12          | 4         |
| 2                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | <b>Rotational, Vibrational and Raman Spectroscopy:</b> Rigid and Non-rigid Rotors. Classification of molecules into spherical, symmetric and asymmetric top category. Selection rule and microwave spectra, Stark effect. Vibrational spectroscopy; Harmonic and Anharmonic Oscillators. Normal coordinates. Effects of Anharmonicity. Vibration-rotation transitions. Raman and Rayleigh scattering – Classical and Quantum Mechanical treatments. Polarization of scattered light. Rotational and Vibrational Raman spectroscopy. Resonance Raman effect. Selection rules of rotational, vibrational and Raman spectroscopy.                                                                                                                                                                                                                                                                                                                                                                                                                                                              | 12          | 4         |
| 3                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | <b>Infrared Spectroscopy (IR):</b> Infrared absorption process, Vibration mode, properties and absorption trends of different chemical bonds, Functional group detection, Analysis of IR spectra, Application of IR spectroscopy; mainly high and low carbonyl stretching, Alkene bond stretching.<br><b>Ultraviolet (UV) and Visible Spectroscopy:</b> Principles of Absorption Spectroscopy: Nature of Electronic Excitations, Origin of UV Band Structure. Chromophore; solvent, structural effects, Woodward-Fieser rules, Woodward's rule, General Application of Ultraviolet Spectroscopy, Polyenes, Carbonyl compounds, Aromatic System, Polycyclic Aromatic hydrocarbons.                                                                                                                                                                                                                                                                                                                                                                                                           | 12          | 4         |
| 4                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | <b>Proton Nuclear Magnetic Resonance Spectroscopy <sup>1</sup>H-NMR:</b> Principles, instrumentation and different techniques (CW and FT) of NMR spectroscopy, factors influencing chemical shift, anisotropic effect, spin-spin interactions, coupling constant (J); Karplus equation, spin-decoupling, NOE, NOE difference spectra. First order and non-first-order splitting, Pople notations. Interpretation of first order spectra of organic molecules. Heteroatom proton; -SH, -NH, -OH, peak broadening, deuterium exchange experiment. Variable Temperature spectra, Application of <sup>31</sup> P, <sup>19</sup> F NMR spectroscopy.<br><b>NMR Spectroscopy:</b> <sup>1</sup> H NMR spectra of paramagnetic coordination compounds, dipolar and contact shifts, magnetic susceptibility and resonance shifts. <sup>11</sup> B, <sup>13</sup> C, <sup>19</sup> F, <sup>27</sup> Al, <sup>31</sup> P, <sup>51</sup> V – NMR spectra. Pascal triangle, Contact shifts. Factors contributing the magnitude of chemical shift. Applications of NMR spectroscopy in inorganic systems. | 12          | 4         |
| 5                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | <b>Electron Spin Resonance Spectroscopy:</b> Basic principles, zero field splitting, and Kramer's degeneracy, factors affecting the 'g' value. Isotropic and anisotropic hyperfine coupling constants, spin Hamiltonian, spin densities and McConnell relationship. Basic instrumentation, measurement techniques and simple applications. Applications of ESR in inorganic complex System and simple SMMs clusters.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        | 12          | 4         |
| <b>Total Contact Hours</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                    |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | <b>60</b>   | <b>20</b> |

**Recommended Books:**

1. Fundamentals of Molecular Spectroscopy by Colin N. Banwell and Elaine M. McCash, 6th Edition
2. Molecular Spectra Vol I by Herzberg, Gerhard
3. Fundamentals of Molecular spectroscopy by P.S. Sindhu
4. Fundamentals of Photochemistry by KK Rohatgi- Mukherjee
5. Principles of Fluorescence Spectroscopy 3rd Edition by Joseph R. Lakowicz
6. Mohan, J. Organic Spectroscopy: Principles and Applications; Alpha Science, 2004.

7. Introduction to Spectroscopy, By Donald L. Pavia, Gary M. Lampman, George S. Kriz, James A. Vyvyan
8. Organic Spectroscopy. W. Kemp
9. Spectroscopic Methods in Organic Chemistry. D. H. Williams and I. Fleming
10. Applications of Absorption Spectroscopy of Organic compounds. J. R. Dyer

| Paper Code: CHEM-DSE-105B                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |                                                                                                                                                                                                                                                                                                                                                                                                                 |             |           |
|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------|-----------|
| <b>Course Title:</b> Molecular Spectroscopy – II<br><b>Contact Hrs:</b> 4 Lectures per Week<br><b>Examination Duration (Hrs.):</b> Two Hours<br><b>Mode of Evaluation:</b><br><b>Continuous Assessment (CA):</b> 10 Marks<br><b>End term Examination (ETE):</b> 40 Marks<br><b>Total Credits:</b> 4<br><b>Semester:</b> I<br><b>Subject Area:</b> Advance Molecular Spectroscopy<br><b>Objective:</b> To acquire advance knowledge about the theory and application of molecular spectroscopy. |                                                                                                                                                                                                                                                                                                                                                                                                                 |             |           |
| Unit                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           | Contents                                                                                                                                                                                                                                                                                                                                                                                                        | Contact Hrs |           |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |                                                                                                                                                                                                                                                                                                                                                                                                                 | L           | T         |
| 1                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | <b>Advance Rotational, Vibrational and Raman Spectroscopy:</b> Thermal Distribution of Quantum States; Intensities in Rotation-Vibration Spectra. Symmetry Properties of the Rotational Levels. Applications of Raman spectroscopy. Details of the related spectrophotometers.                                                                                                                                  | 15          | 5         |
| 2                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | <b>Advance Ultraviolet (UV) and Visible Spectroscopy:</b> Analytical Uses of UV Spectroscopy, Study of Charge Transfer complexes, Use of Sunscreen Dyes, Linearly Polarized Light, Circularly Polarized light, The term (ORD) and (CD)–Chiroptical Properties, UV-vis and Chiroptical Spectroscopy, The Octane rule, Application of (ORD CD) and Octane Rule for Ketones.                                       | 15          | 5         |
| 3                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | <b>Advance Infrared Spectroscopy (IR):</b> Instrumentation, Sample Handling, FTIR, NDIR techniques, Interpretation of Typical Cases-compound Containing Nitrogen, Sulphur and Halogens. IR Radiation and Greenhouse Effect, Infrared Radiation and Automobile Pollutants, The Breath Analyzer Tool.                                                                                                             | 15          | 5         |
| 4                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | <b>Advanced Proton Nuclear Magnetic Resonance Spectroscopy <sup>1</sup>H-NMR:</b> Introduction to pulsed-FT-NMR. Product-operator formalism of 1D and 2D NMR. Determination of three-dimensional structure of molecules using NMR spectroscopy, NOE, NOESY, COSY, Solid state NMR (13C-CP-MAS), Chemical Shift Anisotropy and Cross Polarization, MRI as a diagnostic tool. DEPT <sup>13</sup> C NMR technique. | 15          | 5         |
| <b>Total Contact Hours</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |                                                                                                                                                                                                                                                                                                                                                                                                                 | <b>60</b>   | <b>20</b> |

**Recommended Books:**

1. Fundamentals of Molecular Spectroscopy by Colin N. Banwell and Elaine M. McCash, 6th Edition
2. Molecular Spectra Vol I by Herzberg, Gerhard
3. Fundamentals of Molecular spectroscopy by P.S. Sindhu
4. Fundamentals of Photochemistry by KK Rohatgi- Mukherjee
5. Principles of Fluorescence Spectroscopy 3rd Edition by Joseph R. Lakowicz
6. Mohan, J. Organic Spectroscopy: Principles and Applications; Alpha Science, 2004.
7. Introduction to Spectroscopy, By Donald L. Pavia, Gary M. Lampman, George S. Kriz, James A. Vyvyan
8. Organic Spectroscopy. W. Kemp
9. Spectroscopic Methods in Organic Chemistry. D. H. Williams and I. Fleming
10. Applications of Absorption Spectroscopy of Organic compounds. J. R. Dyer

| Paper Code: CHEM-DSE-105C                                                                                                                                                                                |  |
|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--|
| <b>Course Title:</b> SWAYAM MOOCs Course.<br>To be selected in the Departmental committee meeting by choosing one of the courses offered by the SWAYAM.<br><b>Total Credits:</b> 4<br><b>Semester:</b> I |  |

**Paper Code: CHEM-SEC-106****Course Title:** Techniques in Organic Chemistry**Contact Hrs:** 8 Contact Hours per Week**Examination Duration (Hrs.):** Five Hours**Mode of Evaluation:****Continuous Assessment (CA):** 10 Marks**End term Examination (ETE):** 40 Marks**Total Credits:** 4**Semester:** I**Subject Area:** Skill enhancement in various techniques in Organic Chemistry**Objective:** To acquire knowledge about separation of a binary organic mixture.

| Unit | Contents                                                                                                                                                                                         |
|------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 1    | Separation of a binary organic mixture by column chromatography and characterization. Separation and identification of monosaccharide present in a given polysaccharide by paper chromatography. |

**Recommended Books:**

1. A text book of practical organic chemistry –A. I. Vogel
2. Comprehensive Practical Organic Chemistry: Qualitative Analysis V K Ahluwalia & S. Dhingra.
3. Bansal R. K. Laboratory Manual of Organic Chemistry, Wiley-Eastern.
4. Practical organic Chemistry –Mann and Saunders
5. Vogel A. I. Practical Organic Chemistry, Longman Group Ltd.
6. Nad A. K.; Mahapatra B. and Ghoshal A. An advanced course in practical chemistry, New Central Book Agency (P) Ltd.

## NEP Syllabus: PG 2 Years Chemistry, Semester – II

| Semester     | Course Type        | Paper Code    | Course                        | Credit |
|--------------|--------------------|---------------|-------------------------------|--------|
| II           | DSC                | CHEM-DSC-201  | Organic Chemistry Theory      | 4      |
|              | DSC                | CHEM-DSC-202  | Inorganic Chemistry Theory    | 4      |
|              | DSC                | CHEM-DSC-203  | Physical Chemistry Theory     | 4      |
|              | DSC                | CHEM-DSC-204  | Inorganic Chemistry Practical | 4      |
|              | DSE                | CHEM-DSE-205A | Molecular Spectroscopy-III    | 4      |
|              |                    | CHEM-DSE-205B | Molecular Spectroscopy-IV     |        |
|              |                    | CHEM-DSE-205C | SWAYAM MOOCs Course           |        |
|              | Skill based Course | CHEM-SEC-206  | Synthetic Organic Chemistry   | 4      |
| Total Credit |                    |               |                               | 24     |

**Paper Code: CHEM-DSC-201**

**Course Title:** Organic Chemistry Theory  
**Contact Hrs:** 4 Lectures per Week  
**Examination Duration (Hrs.):** Two Hours  
**Mode of Evaluation:**  
**Continuous Assessment (CA):** 10 Marks  
**End term Examination (ETE):** 40 Marks  
**Total Credits:** 4  
**Semester:** II  
**Subject Area:** Organic Chemistry  
**Objective:** To acquire advance knowledge about the organic reagents, natural product and heterocyclic chemistry.

| Unit                       | Contents                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | Contact Hrs |           |
|----------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------|-----------|
|                            |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        | L           | T         |
| 1                          | <b>Oxidations:</b> Different oxidative processes based on one-electron and two-electron oxidants, oxidations with Cr(VI) oxidants; Collin oxidation, PCC, PDC and others, DMSO-based oxidations: Swern, Moffat, DMSO-SO <sub>3</sub> complex, DMSO-Ac <sub>2</sub> O, Hypervalent iodine oxidations: Dess-Martin periodinate, IBX, iodobenzene diacetate, Oxidation with MnO <sub>2</sub> , Tl(NO <sub>3</sub> ) <sub>3</sub> , Ag <sub>2</sub> O, RuO <sub>4</sub> , Ag(RCOO) <sub>2</sub> and OsO <sub>4</sub> .<br><b>Reductions:</b> Different reductive processes, catalytic hydrogenation; homogenous and heterogeneous, reduction with metal hydrides of B, Al, Sn and Si, catalytic and transfer hydrogenations, dissolving metal reductions, diimide reduction, synthetically useful hydrogenolysis reactions, samarium and indium-based reducing agents, enzymatic and microbial reductions. | 15          | 5         |
| 2                          | <b>Name Reactions/Reagents and Rearrangements:</b> Wittig reactions and various modifications, Peterson elimination, Sharpless asymmetric epoxidation and dihydroxylation, Barton reaction, Hofmann-Löffler-Freytag reaction, Shapiro reaction, Fragmentation reactions; Grob fragmentation, Von-Richter and Smiles rearrangement, Mitsunobu reaction, Yamaguchi and Mukayama esterification, Ohira-Bestmann reagents, Corey-Fuchs Reaction, Olefin metathesis, Nazarov cyclization, Transition metal catalysed organic reactions involving Pd, Ni, Cu, Rh, Ru etc.                                                                                                                                                                                                                                                                                                                                    | 15          | 5         |
| 3                          | <b>Heterocyclic Chemistry:</b> Synthesis, reactivity, and uses of the following compounds and their derivatives: imidazole, pyrazole, oxazole, iso-oxazole, thiazole, iso-thiazole and 5, 6-membered rings containing two heteroatoms, pyrimidines and purines.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        | 15          | 5         |
| 4                          | <b>Chemistry of Natural Products-I:</b> Terpenoids: Introduction, Classification (with proper structural examples of each category), isolation, and structure elucidation of some representative compounds. Biogenesis and biosynthesis of terpenoids.<br>Steroids: Introduction, classification, source of occurrence, brief chemistry of cholesterol, importance and role of steroids in our body, conversion of cholesterol into other bioactive Steroids and chemistry of estrone. Application of natural products in Ayurveda in ancient India.                                                                                                                                                                                                                                                                                                                                                   | 15          | 5         |
| <b>Total Contact Hours</b> |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        | <b>60</b>   | <b>20</b> |

**Recommended Books:**

1. F.A. Carey and R.J. Sundberg, Advanced Organic Chemistry Part A and Part B, 4<sup>th</sup> Edn., Plenum Press, New York
2. March's Advanced Organic Chemistry, 4<sup>th</sup> edition
3. Maya Shankar Singh, Reactive intermediates inorganic Synthesis, Wiley-VCH
4. Carruthers, Modern Methods of Organic Synthesis, Cambridge University Press, 4<sup>th</sup> Edn.
5. Jie Jack Li, Name Reactions, fourth edition, Springer
6. John A. Joule, Keith Mills, Heterocyclic Chemistry, 5<sup>th</sup> edn. Wiley
7. I.L. Finar, volume II
8. K. C. Nicolaou, Eric J. Sorensen, Classics in total synthesis, Wiley-VCH

**Paper Code: CHEM-DSC-202**

**Course Title:** Inorganic Chemistry Theory

**Contact Hrs:** 4 Lectures per Week

**Examination Duration (Hrs.):** Two Hours

**Mode of Evaluation:**

**Continuous Assessment (CA):** 10 Marks

**End term Examination (ETE):** 40 Marks

**Total Credits:** 4

**Semester:** II

**Subject Area:** Inorganic Chemistry

**Objective:** To acquire comprehensive knowledge of organometallic chemistry, magneto chemistry, symmetry and group theory, chemistry of elements, and bioinorganic chemistry.

| Unit                       | Contents                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | Contact Hrs |           |
|----------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------|-----------|
|                            |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | L           | T         |
| 1                          | <b>Organometallics and Catalysis:</b> Reactions of organometallic complexes: substitution, oxidative addition, reductive elimination, insertion and elimination, electrophilic and nucleophilic reactions of coordinated ligands. Catalysis by organometallic compounds: Hydrogenation of olefins, Wilkinson's catalyst, Tolman catalytic loop; synthesis gas, water-gas shift reaction; Hydroformylation (oxo process), Monsanto acetic acid process, Wacker process; synthetic gasoline: Fischer-Tropsch process and Mobile process, polymerization, oligomerization and metathesis reactions of alkenes and alkynes, Ziegler-Natta catalysis, photo dehydrogenation catalyst (platinum POP). Palladium catalyzed C-C, C-N, C-O, C-P and C-S cross coupling reactions.                                                                                    | 12          | 4         |
| 2                          | <b>Magneto Chemistry:</b> Basic principles of magnetism, Magnetic properties, paramagnetism, ferro- and anti-ferromagnetism, diamagnetism, Pascal constants, Curie equation, Russell-Saunders terms, determination of magnetic susceptibility, application of Van-Vleck susceptibility equation, Magnetic properties and coordination compounds Spin and orbital moments, spin-orbit coupling, quenching of orbital moment, spin only formula, room temperature and variable temperature magnetic moments (VTM) and spin crossover. Magnetic properties of first transition series metal ions, lanthanides and actinides, magnetic exchange interactions. Basic Concept of Single Molecule Magnets (SMM), properties and examples of SMMs.                                                                                                                  | 12          | 4         |
| 3                          | <b>Chemistry of Elements:</b><br><b>d-Block Elements:</b> Electronic configuration, oxidation states; aqueous, redox and coordination chemistry, spectral and magnetic properties of compounds in different oxidation states, horizontal and vertical trends in respect of 3d, 4d, and 5d elements with references to Ti-Zr-Hf, V-Nb-Ta, Cr-Mo-W, Mn-Tc-Re and Pt group metals. Occurrence and isolation in respect of V, Mo, W, Re, Pt. Iso- and heteropoly oxometalates with respect to V, Mo, and W: synthesis, reactions, structures, uses, metal-metal bonded dinuclear d-metal complexes (examples), Bonding in dirhenium complexes.<br><b>f-Block Chemistry:</b> Lanthanide and actinide contractions and their consequences, separation of lanthanides and actinides and their applications (examples). Comparison between d and f-block chemistry. | 12          | 4         |
| 4                          | <b>Bioinorganic Chemistry 1</b><br><b>Transport and Storage of Dioxygen:</b> Active site structures and bio functions of O <sub>2</sub> -uptake proteins: haemoglobin, myoglobin, hemocyanin and hemerythrin; model synthetic dioxygen complexes. Chelation-therapy.<br><b>Electron Transfer in Biology:</b> Active site structures and functions of cytochromes, cytochrome; iron-sulfur proteins (ferredoxins). Respiratory electron transport chain, cytochrome c oxidase. Photosynthesis and chlorophylls, photosystem-I and photosystem-II and their roles in cleavage of water. Model systems. Biological and a biological nitrogen fixing systems, model study.                                                                                                                                                                                      | 12          | 4         |
| 5                          | <b>Symmetry and Group Theory:</b> Symmetry elements and symmetry operations, symmetry groups, molecular dissymmetry and optical activity, symmetry point groups for compounds having co-ordination number 2 to 9, matrix representation of groups, reducible and irreducible representation, and the Great orthogonality theorem. Effect of lowering of symmetry on the orbitals and energy levels, correlation table, correlation diagrams, Tanabe-Sugano diagram, Justification of Laporte selection rule, vibronic coupling and vibronic polarization, polarization of electronically allowed transitions. Symmetry adapted linear combinations (SALCs) and the M.O. Description of organic and organometallic molecules.                                                                                                                                | 12          | 4         |
| <b>Total Contact Hours</b> |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | <b>60</b>   | <b>20</b> |

**Recommended Books:**

1. Inorganic Chemistry — Housecroft & Sharpe
2. Advanced Inorganic Chemistry — Cotton & Wilkinson
3. Basic Organometallic Chemistry: Concepts, Syntheses and Applications — B. D. Gupta, A J Elias
4. Principles of Bioinorganic Chemistry— Stephen J. Lippard & Jeremy M. Berg
5. Magnetochemistry—R. L. Carlin & A. J. Van Duyneveldt.
6. Chemical Applications of Group Theory— F. Albert Cotton
7. Elements of Magnetochemistry—R. L. Dutta and A. Syamal
8. Bioinorganic Chemistry —Asim K. Das, M. Das, A. Das & U. Das

**Paper Code: CHEM-DSC-203**

**Course Title:**Physical Chemistry Theory  
**Contact Hrs:** 4 Lectures per Week  
**Examination Duration (Hrs.):** Two Hours  
**Mode of Evaluation:**  
**Continuous Assessment (CA):** 10 Marks  
**End term Examination (ETE):** 40 Marks  
**Total Credits:** 4  
**Semester:**II  
**Subject Area:**Quantum Mechanics, Polymer Chemistry and Biophysical Chemistry  
**Objective:** To acquire knowledge of quantum mechanics, polymer chemistry and biophysical chemistry.

| Unit                       | Contents                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          | Contact Hrs |           |
|----------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------|-----------|
|                            |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | L           | T         |
| 1                          | <b>Quantum Mechanics of Rotational Motion:</b> Angular momentum operators and their commutation relations. Operator algebra and Ladder operators for Rotational motion. Solution of Schrodinger equation using the operator method as well as the technique for solution of differential equation. Quantum Mechanics of rigid rotor and its application. Angular momentum operators and their commutation relations. Operator algebra and Ladder operators for Rotational motion. Solution of Schrodinger equation using the operator method as well as the technique for solution of differential equation. Quantum Mechanics of rigid rotor and its application.                                                                                                                                                | 12          | 4         |
| 2                          | <b>Hydrogen Atom:</b> Separation of translational and internal motion of a two-body problem. Determination of radial part of the wave function. Relation among principal, azimuthal and magnetic quantum number. Nodal properties of angular part as well as the radial part of the Hydrogen atom wavefunction. Shape of the orbitals, Space quantization. Selection rules for Hydrogen atom.                                                                                                                                                                                                                                                                                                                                                                                                                     | 12          | 4         |
| 3                          | <b>Approximate Methods and their Applications:</b> Variation theorem, Linear variation method, Applicability of variation method to excited states. Time-independent perturbation theory for nondegenerate states, Perturbation of a two-level system, Many level systems, Degenerate perturbation theory and their applications, Eckert's Theorem. Hydrogen and Helium atoms. Hellman-Feynman and Virial Theorems. Time-dependent perturbation theory, Rabi Oscillation, Many level system; the variation of constants, the effect of slowly switched constant perturbation, The effect of oscillating perturbation, Transition rates to continuum, Radiation-matter interaction. Fermi Golden rule, Einstein transition probabilities, lifetime and energy uncertainty.                                         | 12          | 4         |
| 4                          | <b>Macromolecules:</b> Definition, Functionality of monomers, Linear polymer, Cross linked polymers, Carothers equation, Monodisperse vs Polydisperse systems, Distribution of molecular weight, Degree of polymerization, Number average, Weight average and Z-average molecular weight.<br><b>Polymer Chemistry-I:</b> Addition and condensation polymerization, kinetic chain length, chain transfer reagent. End to end distance, radius of gyration, Flory-Huggins theory of polymer solution and the entropy, Good and poor solvents, Flory temperature. Determination of molecular weight, Viscosity of macromolecular solution, Viscosity average molecular weight, Osmotic pressure and Number average molecular weight, Light scattering, Sedimentation, Equilibrium and sedimentation velocity method. | 12          | 4         |
| 5                          | <b>Surface Chemistry and Biophysical Chemistry:</b> Surface tension, curved surfaces, Young-Laplace and Kelvin equations. Adsorption on solids, micelles reverse micelles, microemulsion, Thermodynamics of micellization, Application of micelles and microemulsion. Hydrophobic hydration, micelle formation, hydrophobic interaction, stabilization and denaturation of protein. Water structure alteration theory of denaturation of protein, protein-lipid interaction, Transport of ions and small molecules through membranes. Ion channels.                                                                                                                                                                                                                                                               | 12          | 4         |
| <b>Total Contact Hours</b> |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | <b>60</b>   | <b>20</b> |

**Recommended Books:**

1. A text book of Physical Chemistry, volume 5 by K.L Kapoor
2. Introductory Polymer Chemistry by G.S. Misra
3. Polymer Chemistry by Sebastian Koltzenburg, Michael Maskos and Oskar Nuyken
4. Modern Electrochemistry 2A, 2B by John O'M Bockris and Amulya K.N. Reddy.
5. Quantum Mechanics: Concepts and Applications — Nouredine Zettili
6. Principles of Quantum Mechanics — R. Shankar
7. Introductory Quantum Mechanics — Richard L. Liboff
8. Modern Quantum Mechanics — J. J. Sakurai & Jim Napolitano
9. Quantum Mechanics, Vol. 1 & 2 — Cohen-Tannoudji, Diu & Laloë

## Paper Code: CHEM-DSC-204

**Course Title:** Inorganic Chemistry Practical

**Contact Hrs:** 8 Contact Hours per Week

**Examination Duration (Hrs.):** Five Hours

**Mode of Evaluation:**

**Continuous Assessment (CA):** 10 Marks

**End term Examination (ETE):** 40 Marks

**Total Credits:** 4

**Semester:** II

**Subject Area:** Inorganic Chemistry Laboratory Work

**Objective:** To acquire practical knowledge about quantitative analyses of inorganic compounds and preparation of inorganic complex.

| Unit | Contents                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |
|------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 1    | <p><b>Synthesis and Spectroscopic Analysis of Metal Complexes:</b> Preparation and FTIR and UV–Visible spectroscopic characterization of coordination compounds including bis(ethylene)nickel(II) thiosulfate; tris(acetylacetonato) complexes of Mn(III), Al(III), Fe(II), and Cu(II); hexamminecobalt (III) chloride; mercury tetrathiocyanatocobaltate(II); Reinecke's salt; copper(II)–biguanide complex; Mn<sub>12</sub> acetate single-molecule magnet; cis- and trans-bis(glycinato)copper(II); and Schiff base complexes such as N,N'-bis(salicylidene)ethylenediamine (salen) with Co(II) and Mn(II).</p>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |
| 2    | <p><b>Analysis of Complex Materials:</b> Estimation of individual components using spectrophotometric techniques, including Fe(III) as [Fe(SCN)]<sup>2+</sup> and Fe(II) as [Fe(phen)<sub>3</sub>]<sup>2+</sup> complexes, Mn as MnO<sub>4</sub><sup>-</sup>, and phosphate as phosphomolybdate blue complex.</p> <p>Quantitative analysis of complex materials such as ores, minerals, metals, alloys, and industrial samples using conventional and instrumental methods, including microwave digestion techniques.</p> <p><b>Spectrophotometric Estimations (Model Samples):</b> Ores and minerals/concentrates such as dolomite (CaCO<sub>3</sub>, MgCO<sub>3</sub>, Fe<sub>2</sub>O<sub>3</sub>, SiO<sub>2</sub>), pyrolusite (MnO<sub>2</sub>, MnO, Fe<sub>2</sub>O<sub>3</sub>), chalcopyrite (CuS, FeS), bauxite (Al<sub>2</sub>O<sub>3</sub>, Fe<sub>2</sub>O<sub>3</sub>, TiO<sub>2</sub>, SiO<sub>2</sub>), chromite (Cr<sub>2</sub>O<sub>3</sub>, Fe<sub>2</sub>O<sub>3</sub>, MnO, SiO<sub>2</sub>), and basic slag (Al<sub>2</sub>O<sub>3</sub>, Fe<sub>2</sub>O<sub>3</sub>, P<sub>2</sub>O<sub>5</sub>, SiO<sub>2</sub>).</p> <p>Metals and alloys including brass (Cu, Zn), solder/type metal (Pb, Sb, Sn), bronze (Cu, Zn, Sn), aluminium bronze (Cu, Al, Fe, Mn), and steel (Cr, Mn, Ni, P).</p> <p>Binary mixtures such as Cr(III)–Mn(II), Fe(III)–Cu(II), and Fe(III)–Al(III).</p> <p>At least one ore/mineral/concentrate and one alloy are to be analyzed during laboratory sessions.</p> <p><b>Analysis of Inorganic Complexes:</b> Studies on the composition of complexes using mole-ratio, slope-ratio, and Job's method of continuous variation (Job's plot).</p> <p>Determination of metal–ligand stability constants through pH-metric and spectrophotometric methods, including systems such as Cu<sup>2+</sup>–glycine complex formation.</p> <p>Measurement of magnetic moments for structural elucidation and determination of electronic configurations.</p> <p>Spectroscopic investigations of DNA–metal complex interactions.</p> |

### Recommended Books:

1. Handy lab manual of inorganic chemistry by Dr. Gurjeet Gujral
2. Advanced Practical Chemistry by Raghupati Mukhopadhyay & Pratul Chatterjee
3. Hand Book of Inorganic Analysis by G. N. Mukherjee
4. Vogel's TEXTBOOK OF QUANTITATIVE CHEMICAL ANALYSIS by G H Jeffery, J Bassett, J Mendham, R C Denney
5. Advanced Practical Chemistry by Subhas C Das

**Paper Code: CHEM-DSE-205A**

**Course Title:** Molecular Spectroscopy – III

**Contact Hrs:** 4 Lectures per Week

**Examination Duration (Hrs.):** Two Hours

**Mode of Evaluation:**

**Continuous Assessment (CA):** 10 Marks

**End term Examination (ETE):** 40 Marks

**Total Credits:** 4

**Semester:** II

**Subject Area:** Molecular Spectroscopy

**Objective:** To acquire knowledge about the theory and application of molecular spectroscopy.

| Unit                       | Contents                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | Contact Hrs |           |
|----------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------|-----------|
|                            |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       | L           | T         |
| 1                          | <b>Electronic Spectroscopy:</b> Diatomic molecules, Rotational and vibrational structures of diatomic electronic transitions. Franck-Condon principle. Dissociation, photodissociation and Predissociation. Chromophores. Vibronic transitions. Spin-orbit coupling and singlet - triplet transitions. Selection rules for molecular electronic transitions. Photoelectron spectroscopy. Excitation of molecules - Singlet and Triplet states. Radiative and Non-radiative relaxations. Absorption, emission and excitation spectra - mirror symmetry. Quenching of Fluorescence. Excited state processes - proton transfer, electron transfer and energy transfer. Marcus Theory. Solvent effect in spectroscopy. Stimulated emission of radiation. Principles of Laser action and its applications. | 10          | 4         |
| 2                          | <b>Resonance Spectroscopy:</b> Nuclear magnetic moment and response in an external magnetic field. Classical and Quantum Mechanical perspectives of nuclear magnetic resonance (NMR). Spin-spin and spin-lattice relaxation and spectral shapes. Chemical shift and nuclear shielding. Spin magnetic moment of electrons and electron spin resonance signal (ESR). g-factor and hyperfine splitting - interaction between nuclear spin and electron spin. Nuclear quadrupole resonance.                                                                                                                                                                                                                                                                                                               | 10          | 3         |
| 3                          | <b>Thermal Analyses:</b> Principle and application of TGA, DTA and DSC spectroscopy in different inorganic systems.<br><b>Mossbauer Spectroscopy:</b> Principle of Mossbauer Spectroscopy. Application of Mossbauer Spectroscopy – Chemical Shift, Quadrupole effect, effect of Magnetic Field, information of spin and oxidation states, structure and bonding, spin transition from spectra of different Mossbauer active nuclei in varieties of environments, Application of Mossbauer spectroscopy in inorganic complex chemistry.                                                                                                                                                                                                                                                                | 10          | 3         |
| 4                          | <b>Carbon -13 NMR Spectroscopy (<sup>13</sup>C-NMR):</b> <sup>13</sup> C-Chemical Shifts, correlation charts, Proton-Coupled, Proton-Decoupled, Off- Resonance Decoupling spectra. Cross Polarization: Origin of the Nuclear Overhauser Effect. APT, DEPT spectra.<br><b>NMR Techniques:</b> Introduction of Two-Dimensional Spectroscopic Methods: Pulse Sequences, Pulse Widths, Spins, and Magnetization Vectors. Application COSY ( <sup>1</sup> H- <sup>1</sup> H), HETCOR ( <sup>13</sup> C- <sup>1</sup> H), HSQC ( <sup>1</sup> H- <sup>13</sup> C), HMQC( <sup>1</sup> H- <sup>13</sup> C), HMBC, TOCSY, SECSY, INADEQUATE, NOESY, ROESY. Determination of relative and absolute stereochemistry.                                                                                            | 12          | 4         |
| 5                          | <b>Mass Spectrometry:</b> Principles, instrumentation and applications of mass spectrometry – methods of generation of ions in EI, CI, FD, FAB, ESI, and MALDI-TOF. Detection of ions, ion analysis, ion abundance, molecular ion peak, metastable peak, isotope, ion-molecule, Interaction and analysis of fragmentation patterns. Calculation MF from mass.                                                                                                                                                                                                                                                                                                                                                                                                                                         | 8           | 2         |
| 6                          | <b>X-ray Crystallography:</b> Fundamentals of X-ray crystallography, crystal forms, lattice, primitive cell, crystal systems and symmetry, non-primitive lattices, crystal classes, space groups, crystals and their properties, Diffraction of X-ray, lattice planes, indices, Bragg's condition, reciprocal lattice, Bragg's law in reciprocal, Geometric data collection (simple examples), structure factor, systematic absence, heavy atom method. Fourier synthesis, Patterson function, experimental diffraction methods (Laue method, rotating crystal method).<br><b>Methods of Growing Single Crystals:</b> Data collection, structure solution, structure refinement, R-values and Goodness of fit.                                                                                        | 12          | 4         |
| <b>Total Contact Hours</b> |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       | <b>60</b>   | <b>20</b> |

**Recommended Books:**

1. Fundamentals of Molecular Spectroscopy by Colin N. Banwell and Elaine M. McCash, 6th Edition
2. Molecular Spectra Vol I by Herzberg, Gerhard
3. Fundamentals of Molecular spectroscopy by P.S. Sindhu
4. Fundamentals of Photochemistry by KK Rohatgi- Mukherjee
5. Principles of Fluorescence Spectroscopy 3rd Edition by Joseph R. Lakowicz

6. Organic Structures from 2D NMR Spectra, L. D. Field, H. L. Li, A. M. Magill.
7. Mass Spectrometry Application to Organic Chemistry. K. Biemann.
8. Spectrometric Identification of Organic Compounds R. M. Silverstein & F. O. Webster; 6<sup>th</sup> edition

| Paper Code: CHEM-DSE-205B                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |                                                                                                                                                                                                                                                                                                                                                                                                                      |             |           |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------|-----------|
| <b>Course Title:</b> Molecular Spectroscopy – IV<br><b>Contact Hrs:</b> 4 Lectures per Week<br><b>Examination Duration (Hrs.):</b> Two Hours<br><b>Mode of Evaluation:</b><br><b>Continuous Assessment (CA):</b> 10 Marks<br><b>End term Examination (ETE):</b> 40 Marks<br><b>Total Credits:</b> 4<br><b>Semester:</b> II<br><b>Subject Area:</b> Advance Molecular Spectroscopy<br><b>Objective:</b> To acquire advance knowledge about the theory and application of molecular spectroscopy. |                                                                                                                                                                                                                                                                                                                                                                                                                      |             |           |
| Unit                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            | Contents                                                                                                                                                                                                                                                                                                                                                                                                             | Contact Hrs |           |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |                                                                                                                                                                                                                                                                                                                                                                                                                      | L           | T         |
| 1                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | <b>Excited State Process:</b> Photophysical processes, static and dynamic quenching, excimers and exciplexes, Energy transfer, charge transfer and dynamics, few examples of donor acceptor pairs. Solvation dynamics. Non-linear optical processes. Photochemical processes and examples                                                                                                                            | 12          | 4         |
| 2                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | <b>Methods and Instrumentations:</b> Steady state absorption spectroscopy, Steady state emission spectroscopy, Time correlated single photon counting                                                                                                                                                                                                                                                                | 12          | 4         |
| 3                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | <b>Advanced <math>^{13}\text{C}</math> NMR Spectroscopy:</b> Calculation of chemical shifts of alkanes, alkenes and alkynes. Homonuclear ( $^{13}\text{C}$ , $^{13}\text{C}$ J) and heteronuclear ( $^{13}\text{C}$ , $^1\text{H}$ J and $^{13}\text{C}$ , $^2\text{H}$ J) coupling. $^{13}\text{C}$ -NMR spectral editing techniques: principle and applications of APT, INEPT and DEPT methods.                    | 12          | 4         |
| 4                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | <b>Advanced Mass Spectrometry:</b> Mass Analysers: Quadrupole, Ion traps, Time of flight (TOF) mass analysers Mass Spectrometry / Mass Spectrometry: Tandem Mass Spectrometry, Instrumentation, Applications. Hyphenated Techniques: GC-MS Principle, instrumentation, LC-MS, ICP – MS - Principal Instrumentation, and Applications, Desorption ionization methods, Spectroscopic Solutions of Structural Problems. | 12          | 4         |
| 5                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | <b>Some Characterization Method:</b> Elemental Analysis (Surface and Bulk), Low and Wide angle XRD, SEM – EDAX, TEM, TG/DTA, TPD-NH <sub>3</sub> , TG-MS, BET-Surface area, FT-IR, Raman, ESR, UV-Vis., XPS, MASNMR, and Cyclic voltammetry.                                                                                                                                                                         | 12          | 4         |
| <b>Total Contact Hours</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |                                                                                                                                                                                                                                                                                                                                                                                                                      | <b>60</b>   | <b>20</b> |

**Recommended Books:**

1. Fundamentals of Molecular Spectroscopy by Colin N. Banwell and Elaine M. McCash, 6th Edition
2. Molecular Spectra Vol I by Herzberg, Gerhard
3. Fundamentals of Molecular spectroscopy by P.S. Sindhu
4. Fundamentals of Photochemistry by KK Rohatgi- Mukherjee
5. Principles of Fluorescence Spectroscopy 3rd Edition by Joseph R. Lakowicz
6. Organic Structures from 2D NMR Spectra, L. D. Field, H. L. Li, A. M. Magill.
7. Mass Spectrometry Application to Organic Chemistry. K. Biemann.
8. Spectrometric Identification of Organic Compounds R. M. Silverstein & F. O. Webster; 6<sup>th</sup> edition

| Paper Code: CHEM-DSE-205C                                                                                                                               |  |
|---------------------------------------------------------------------------------------------------------------------------------------------------------|--|
| <b>Course Title:</b> SWAYAM MOOCs Course.<br>To be selected in the Departmental committee meeting by choosing one of the courses offered by the SWAYAM. |  |
| <b>Total Credits:</b> 4<br><b>Semester:</b> II                                                                                                          |  |

**Paper Code: CHEM-SEC-206****Course Title:** Synthetic Organic Chemistry**Contact Hrs:** 8 Contact Hours per Week**Examination Duration (Hrs.):** Five Hours**Mode of Evaluation:****Continuous Assessment (CA):** 10 Marks**End term Examination (ETE):** 40 Marks**Total Credits:** 4**Semester:** II**Subject Area:** Skill enhancement on various methods in Organic Chemistry.**Objective:** To acquire practical knowledge about synthesis of organic compounds (single as well as multistep).

| Unit | Contents                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |
|------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 1    | <p><b>Studies Single Step Synthesis:</b></p> <ol style="list-style-type: none"><li>1. 1,2-Phenylindole (Fischer indole synthesis)</li><li>2. 7-Hydroxy-3-methylflavone (Baker-Venkatraman reaction)</li><li>3. Benzyl alcohol and benzoic acid from benzaldehyde (Cannizzaro reaction)</li><li>4. 4-Chlorotoluene from <i>p</i>-toluidine (Sandmeyer reaction)</li><li>5. Benzilic acid from benzoin (Benzilic acid rearrangement)</li><li>6. Benzopinacol (Photochemical reaction)</li><li>7. 7-Hydroxy-4-methylcoumarin (Pechmann Reaction)</li><li>8. Benzanilide (Beckmann rearrangement)</li><li>9. Vanillyl alcohol from vanillin (NaBH<sub>4</sub> reduction)</li><li>10. 2-and 4-nitrophenols (nitration and separation by steam distillation)</li><li>11. Stilbene from benzyl chloride (Wittig reaction)</li><li>12. Ethyl cinnamate from benzaldehyde (Wittig reaction)</li><li>13. Triphenyl or diphenylmethyl carbinol (Grignard reaction)</li><li>14. Benzotriazole</li><li>15. 1-Phenyl-3-methylpyrazol-5-one</li><li>16. 2,4-diethoxycarbonyl-3,4-dimethylpyrrole from methylacetoacetate</li><li>17. Quinoline from aniline (Skraup synthesis)</li><li>18. 1-phenylethanol from acetophenone (LAH reduction)</li><li>19. Biginelli synthesis of dihydropyrimidones</li><li>20. Binaphol synthesis</li><li>21. Benzylidene acetone</li><li>22. Acetylation of aniline by Zn and acetic acid</li></ol> <p>Or, any suitable organic transformation based on available facilities</p> <p><b>Multistep Synthesis:</b></p> <ol style="list-style-type: none"><li>1. 4-Nitrotoluene → 4-nitrobenzoic acid → 4-Aminobenzoic acid</li><li>2. Cyclohexanone → Phenylhydrazone → 1,2,3,4-tetrahydrocarbazole</li><li>3. Phthalimide → N-benzylphthalimide → benzylamine</li><li>4. O-nitroaniline → O-phenylenediamine → Benzimidazole</li><li>5. Phthalic acid → phthalimide → Anthranilic acid</li><li>6. Benzylcyanide → p-Nitrobenzylcyanide → p-Nitrophenylacetic acid</li><li>7. Cyclohexanone → Enamine → 2-acetylcyclohexanone</li></ol> <p><b>Note:</b> At least ten single step and three multi step synthesis should be carried out.</p> |

**Recommended Books:**

1. Comprehensive Practical Organic Chemistry by V. K. Ahluwalia and Renu Aggarwal
2. Monograph on Green Chemistry Laboratory Experiments by Green Chemistry Task Force Committee, DST
3. A text book of practical organic chemistry. A. I. Vogel

## NEP Syllabus: PG 2 Years Chemistry, Semester – III

| Semester            | Course Type                                     | Paper Code           | Course                                                                    | Credit    |
|---------------------|-------------------------------------------------|----------------------|---------------------------------------------------------------------------|-----------|
| III                 | DSC                                             | <b>CHEM-DSC-301</b>  | Physical Chemistry Theory                                                 | 4         |
|                     | DSE                                             | <b>CHEM-DSE-302A</b> | Organic Chemistry Theory                                                  | 4         |
|                     |                                                 | <b>CHEM-DSE-302B</b> | Advance Organic Chemistry Theory                                          |           |
|                     | DSE                                             | <b>CHEM-DSE-303A</b> | Inorganic Chemistry Theory                                                | 4         |
|                     |                                                 | <b>CHEM-DSE-303B</b> | Supramolecular Chemistry, Crystal Engineering and Inorganic Nanomaterials |           |
|                     |                                                 | <b>CHEM-DSE-303C</b> | SWAYAM MOOCs Course                                                       |           |
|                     | Advance Research Methodology                    | <b>CHEM-DRP-304</b>  | Advance Research Methodology                                              | 4         |
|                     | Dissertation/Research Project/ Entrepreneurship | <b>CHEM-DRP-305</b>  | Dissertation/Research Project/Entrepreneurship                            | 8         |
| <b>Total Credit</b> |                                                 |                      |                                                                           | <b>24</b> |

**Paper Code: CHEM-DSC-301**

**Course Title:**Physical Chemistry Theory  
**Contact Hrs:** 4 Lectures per Week  
**Examination Duration (Hrs.):** Two Hours  
**Mode of Evaluation:**  
**Continuous Assessment (CA):** 10 Marks  
**End term Examination (ETE):** 40 Marks  
**Total Credits:** 4  
**Semester:**III  
**Subject Area:**Quantum Mechanics, Statistical Mechanics, Irreversible Thermodynamics and Solid State Chemistry  
**Objective:** To acquire knowledge of quantum theory, statistical mechanics, irreversible thermodynamics and solidstate chemistry.

| Unit                       | Contents                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            | Contact Hrs |           |
|----------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------|-----------|
|                            |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | L           | T         |
| 1                          | <b>Spin and Many Electron Wavefunctions:</b> Introduction to spin. Operator algebra for spin. Construction of matrix representation of spin operators, Eigenvalues and eigenfunctions of spin operators. Non-relativistic wavefunction for Hydrogen atom. Many-electron wavefunctions-examples with 2 and 3 electron systems, Slater determinants. Projection Operators. Parity Operator and Pauli Principle, The Pauli exclusion principle. Introduction of core, Coulomb, and exchange integrals with their properties- example of He atom.                                                                                                                                                                                       | 12          | 4         |
| 2                          | <b>Connection between Thermodynamics and Statistical Mechanics:</b> Definition of Microstates and Macrostates. Boltzmann's definition of entropy. Formula for calculation of thermodynamic properties in terms of number of microstates. Determination of number of microstates for classical ideal gas. Connection among the properties of ideal gas, Gibbs paradox, Sackur-Tetrode equation.                                                                                                                                                                                                                                                                                                                                      | 12          | 4         |
| 3                          | <b>Ensemble Method and its Application:</b> Definition of ensemble. A priori probability. Gibbs postulate in Statistical mechanics. Ergodic hypothesis. Prescription for studying of thermodynamic systems based on ensemble method. Preparation of equilibrium ensemble corresponding to given thermodynamic system (isolated, closed and open). Partition function. Calculation of thermodynamic properties in terms of partition function. Theory of Fluctuations. Calculation of fluctuation in energy, number of particles, density, entropy, volume, temperature etc.                                                                                                                                                         | 12          | 4         |
| 4                          | <b>Irreversible Thermodynamics:</b> Thermodynamic criteria for Non-equilibrium states. Entropy production and Entropy balance equations. Generalized flux and forces. Stationary states. Phenomenological equations. Microscopic reversibility and Onsager equation. Applications in physico-chemical and biological phenomena. Coupled reactions.                                                                                                                                                                                                                                                                                                                                                                                  | 12          | 4         |
| 5                          | <b>Solid State Chemistry:</b> Crystalline and amorphous structures. Reciprocal lattice concept, Brillouin zones, and their importance in electron energy levels, Bravais lattices, Miller indices, interplanar spacing, and unit cell calculations, Crystal Defects: Point defects (Schottky, Frenkel), non-stoichiometric defects (metal excess/deficiency), and F-centers, Electrical & Magnetic Properties: Band theory - Quantum mechanical aspect (Metals, Insulators, Semiconductors), Semiconductor Hall effect and Hall co-efficient, Bloch's Theorem and the Drude Model, Dielectric properties, and Magnetic properties of solids, Dia-, para-, ferro-, ferri-, and antiferromagnetism, Bragg's law and structure factor. | 12          | 4         |
| <b>Total Contact Hours</b> |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | <b>60</b>   | <b>20</b> |

**Recommended Books:**

1. Quantum Chemistry by Donald A McQuarrie
2. Quantum Mechanics second edition, by V. Devanathan
3. Quantum Chemistry fifth edition by Ira N. Levine
4. Atkins' Physical Chemistry tenth edition by Peter Atkins and Julio de Paula
5. A text book of Physical Chemistry, Quantum chemistry and Molecular Spectroscopy, volume 4 by K.L Kapoor
6. A text book of Physical Chemistry, volume 5 by K.L Kapoor
7. Chemical Thermodynamics J. Rajaram and J.C. Kuriacose
8. Principles of Solid State by H.V Keer
9. Solid State Physics by A J Dekker
10. Solid State Physics second edition by J.R. Hook & H.E. Hall
11. Statistical Mechanics by Donald A McQuarrie
12. Statistical Mechanics by RK Pathria
13. Statistical Mechanics: Principles and Selected Applications by Terrell L. Hill

| Paper Code: CHEM-DSE-302A                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |             |           |
|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------|-----------|
| <b>Course Title:</b> Organic Chemistry Theory<br><b>Contact Hrs:</b> 4 Lectures per Week<br><b>Examination Duration (Hrs.):</b> Two Hours<br><b>Mode of Evaluation:</b><br><b>Continuous Assessment (CA):</b> 10 Marks<br><b>End term Examination (ETE):</b> 40 Marks<br><b>Total Credits:</b> 4<br><b>Semester:</b> III<br><b>Subject Area:</b> Organic Chemistry<br><b>Objective:</b> To acquire knowledge about natural product, carbohydrate chemistry, green chemistry, and photochemistry. |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |             |           |
| Unit                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | Contents                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          | Contact Hrs |           |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | L           | T         |
| 1                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | <b>Chemistry of Natural Products – II</b><br><b>Alkaloids:</b> Introduction, general methods of isolation and structure elucidation, structure and synthesis of ephedrine, nicotine and papaverine. Structure and stereochemistry and medicinal importance of alkaloids of quinine and morphine group (cinchona and opium alkaloids).<br><b>Natural Antioxidants:</b> Chemistry of naturally occurring oxygen heterocycles, polyphenolics and other antioxidants. Use of some natural products in ayurveda as medicines in ancient India.                                                                                                                                                                                                                                                         | 15          | 5         |
| 2                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | <b>Green Chemistry:</b> Green Chemistry-Overview, Set of Principles of Green Chemistry, Green synthetic methods, Catalytic methods, Organic synthesis in aqueous media, Ionic liquid, Supercritical fluids and microwave, Solvent free organic reactions, solid phase organic synthesis.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          | 15          | 5         |
| 3                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | <b>Carbohydrate Chemistry:</b> Basic structure and type of sugars; Conformational analysis of monosaccharides (pentoses and hexoses). Protection and deprotection. <i>O</i> -glycosylation, <i>C</i> -glycosylation. Deoxysugars, amino sugars, glycal sugars and their synthetic aspects. Carbohydrates as chiral pools inorganic synthesis; Synthesis of medicinally important heterocycles derives from carbohydrates.                                                                                                                                                                                                                                                                                                                                                                         | 15          | 5         |
| 4                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | <b>Photochemistry:</b> Basic principles, Jablonski diagram, photochemistry of olefin compounds – <i>Cis/trans</i> isomerization stereomutation, photo chemistry of carbonyl compounds–Norrish Type I and Norrish Type II cleavages, photoreduction, H-atom abstraction, photocyclo addition to ketones, ethylenes, Paterno-Büchireaction, photochemistry of unsaturated ketones, esters, acids, benzoquinones, nitrite, photo fries rearrangement, Barton reaction. <i>di-pi</i> -methane rearrangement, photochemistry of arenes, Photoreaction in solid state. Method of generation and detection of radicals (ESR), radical initiators, reactivity pattern of radicals, substitution and addition reactions involving radicals, cyclisation of radicals, allylic halogenation, auto-oxidation. | 15          | 5         |
| <b>Total Contact Hours</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | <b>60</b>   | <b>20</b> |

**Recommended Books:**

1. CRC Handbook of Organic Photochemistry and Photobiology. Two Volume Set-CRC Press. Axel Griesbeck, Michael Oelge möller, Francesco Ghetti.
2. Introduction To Organic Photochemistry-Wiley. J. D. Coyle.
3. Organic Photochemistry. Principles and Applications-Academic Press. Jacques Kagan.
4. GREENE'S PROTECTIVE GROUPS IN ORGANIC SYNTHESIS, PETERG. M.WUTS, and THE ODORAW. GREENE Wiley-Inter science
5. Organic Synthesis with Carbohydrates, GEERT-JANBOONS, Sheffield Academic Press, Blackwell
6. The Organic Chemistry of Sugars, Edited by Daniel E. Levy Péter Fügedi, CRC

**Paper Code: CHEM-DSE-302B**

**Course Title:** Advance Organic Chemistry Theory

**Contact Hrs:** 4 Lectures per Week

**Examination Duration (Hrs.):** Two Hours

**Mode of Evaluation:**

**Continuous Assessment (CA):** 10 Marks

**End term Examination (ETE):** 40 Marks

**Total Credits:** 4

**Semester:** III

**Subject Area:** Advance Organic Chemistry

**Objective:** To acquire advanced knowledge about the most important bio-molecules and medicinal chemistry.

| Unit                       | Contents                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | Contact Hrs |           |
|----------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------|-----------|
|                            |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       | L           | T         |
| 1                          | <b>Pharmaceuticals:</b> Introduction to the clinically used drugs such as sulphonamides, antimalarials, arsenical drugs, antibiotics, the penicillin's, cephalosporin C, streptomycin, chloramphenicol, macrolide group of antibiotics, polypeptide antibiotics. General pharmacology, qualitative aspects of drug action, receptors, quantitative aspects of drug-receptor interactions, therapeutic index, various modes of administration of drugs, gram positive and negative micro-organisms, NSAID's and their mode of action. Representative antibacterial drugs, anticancer, anti-HIV drugs, their structure mode of action.                                                                                                                                                                                                                                                                                                                                                  | 15          | 5         |
| 2                          | <b>Enzymes, Coenzymes, Fermentation:</b> Enzymes- classification, mode of action, key features of active site, Chymotrypsin, Trypsin, Elastase, Michaelis-Menten model for kinetic properties of enzymes, enzymic inhibition-competitive and non-competitive. Enzymic oxidation of simple biomolecules. Cyclodextrin as Enzyme Mimics, Synzymes Cofactor, Apoenzyme, Holoenzyme, Prosthetic group, Coenzymes- catalytic role of TPP, COASH, coenzyme-I, coenzyme-II, AMP, ADP, ATP, FMN, FAD, NAD <sup>+</sup> , NADP <sup>+</sup> , NADH, NADPH, PLP, and other high energy molecules, their biogenetics, coupled reactions.                                                                                                                                                                                                                                                                                                                                                         | 15          | 5         |
| 3                          | <b>Proteins and Peptides:</b> General nature, characteristics, introduction to primary, secondary and tertiary structures. Solid Phase Peptide Synthesis: using Wang, 2-CTC, Rinkamide, Sieber amide resin. Ramachandran Plot. Separation and Purification Methods: Electrophoresis, isoelectric focusing, gel filtration, affinity chromatography, and ion exchange – choice of gel support materials (agarose, cellulose, polyacrylamide, glass beads, DEAE-cellulose, CM-cellulose etc.) HLC.<br><b>Fragmentation of Polypeptides:</b> Chemical Methods – cleavage of di-sulfide bonds; oxidation; partial acid hydrolysis; cleavages at methionine, tryptophan, tyrosine, cysteine Enzymic Methods – protein modification reactions disulphide bond cleavage, alkylation of sulphhydryl groups, modification of lysine and arginine residues. Specificity and conditions for trypsin, thrombin, chymotrypsin, thermolysin, pepsin papain etc. Determination of Peptide Sequences. | 15          | 5         |
| 4                          | <b>Nucleic Acids:</b> Human Genome project, Structure and synthesis of nucleosides and nucleotides, DNA, RNA, PNA, LNA, Solid phase synthesis of DNA. DNA sequencing, replication of DNA, Transcription, Translation, mutation, genetic code, role of nucleic acid in the biosynthesis of proteins, Har Gobind Khorana Codon Chart, DNA finger printing, DNA breathing, DNA Modification and chemical carcinogenesis, P. C. reactions.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | 15          | 5         |
| <b>Total Contact Hours</b> |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       | <b>60</b>   | <b>20</b> |

**Recommended Books:**

1. Stryer L., Berg J.M. and Tymoczko J. L. "Biochemistry", W. H. Freeman & Co. NY.
2. Nelson D. L. and Cox M. M., "Lehninger Principles of Biochemistry" W. H. Freeman & Company. NY.
3. Mann J., "Chemical Aspects of Biosynthesis", Oxford Univ. Press.

**Paper Code: CHEM-DSE-303A**

**Course Title:** Inorganic Chemistry Theory

**Contact Hrs:** 4 Lectures per Week

**Examination Duration (Hrs.):** Two Hours

**Mode of Evaluation:**

**Continuous Assessment (CA):** 10 Marks

**End term Examination (ETE):** 40 Marks

**Total Credits:** 4

**Semester:** III

**Subject Area:** Inorganic Chemistry

**Objective:** To acquire comprehensive knowledge of inorganic rings, cages, and clusters; nuclear chemistry and radiochemical analysis; advanced bioinorganic chemistry; inorganic reaction mechanisms; and electrochemical analysis techniques.

| Unit                       | Contents                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         | Contact Hrs |           |
|----------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------|-----------|
|                            |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | L           | T         |
| 1                          | <b>Inorganic Rings, Cages and Clusters:</b> Stereochemistry and bonding in non-transition element compounds, Cages, clusters, rings – boranes, carboranes, metalloboranes and metallocarboranes, siloxanes, hetero-atomic rings, phosphonitrilic compounds. Metal-metal bonding (M.O. Approach), metal-metal single and multiple bonded compounds. Low nuclearity (M3, M4) and high nuclearity (M5-M10) carbonyl clusters: skeletal electron counting, Wade-Mingos-Louhrrule, Jemmisrule. Application of isolobal and isoelectronic relationships, Nb and Ta clusters, Mo and W clusters. Cluster compounds in catalysis.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        | 12          | 4         |
| 2                          | <b>Nuclear Chemistry &amp; Radiochemical Analysis:</b><br><b>Nuclear models:</b> Nuclear stability, terrestrial abundance and distribution, relativistic effect, electronic configuration, oxidation states, aqueous-redox- and complex-chemistry; Nuclear forces, liquid drop model, shell model; Fermi gas model; magic numbers, nuclear spin and nuclear isomerism. Nuclear reactions: Energetics, mechanism and models of nuclear reactions. Nuclear fission and nuclear fusion, fission products and fission yields. Interactions of radiation with matters, chemical effects of nuclear transmutation (elementary idea), Nuclear reactors and particle accelerators.<br><b>Radioactive Techniques:</b> Detection and measurement of radiation- GM ionization and proportional counters. Study of chemical reactions by tracer techniques, isotope exchange and kinetic isotope effect. Radiometric analysis: Isotope dilution analysis, age determination, neutron activation analysis (NAA) and their applications. Radiation hazards and safety measures.                                                                                                | 12          | 4         |
| 3                          | <b>Advanced Bioinorganic Chemistry 2:</b> Metal ion interactions with purine and pyrimidine bases, nucleosides, nucleotides and nucleic acids, DNA and RNA, metal ions in genetic information transfer.<br><b>Redox enzymes:</b> Catalase, peroxidase, super oxide dismutase (SOD), cytochrome P-450, nitric oxide synthases (NOS), ascorbate oxidase, aldehyde oxidase; molybdo enzymes: xanthenes oxidase, nitrate reductase, sulphite oxidase including some model study.<br><b>Vitamins and coenzymes:</b> Vitamin B6 and vitamin B12 coenzymes, model systems;<br><b>Supramolecular chemistry:</b> Metal in medicine: anticancer drugs.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | 12          | 4         |
| 4                          | <b>Inorganic Reaction Mechanism:</b> Mechanism of substitution reactions, solvent exchange, aquation, anation, base hydrolysis, acid catalyzed aquation, pseudo-substitution. Energy profile diagram of ligand substitution reactions- associative (A), dissociative (D), interchange (I) etc. type pathways, relation between intimate and stoichiometric mechanisms of ligand substitution, some important rate laws, activation parameters ( $\Delta S^\ddagger$ , $\Delta H^\ddagger$ , $\Delta V^\ddagger$ ), mechanism of isomerization reaction-linkage isomerism, cis-trans isomerism, intramolecular and intermolecular racemization, Ray-Dutt and Bailar twist mechanisms, substitution in octahedral complexes- the Eigen-Wilkins mechanism, the Fuoss-Eigen equation, linear free energy relation (LFER) etc.<br><b>Mechanism of electron transfer reactions:</b> General characteristics and classification of redox reactions, self-exchange reactions. Frank-Condon principle (non-mathematical treatment). Outer sphere and Inner sphere reactions, applications of Marcus expression (simple form), and redox catalyzed substitution reactions. | 12          | 4         |
| 5                          | <b>Electrochemical analyses:</b> Introduction to electrochemical methods, electrochemical cells, diffusion controlled limiting current, voltage scanning polarography, shape and interpretation of polarographic wave, current-voltage relationship during electrolysis. Principles and applications of voltammetry, cyclic voltammetry, polarography, anodic stripping voltammetry, amperometry, coulometry, electro-gravimetry. Spectro-electrochemistry, Hyphenated techniques; Fuel cells.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | 12          | 4         |
| <b>Total Contact Hours</b> |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | <b>60</b>   | <b>20</b> |

**Recommended Books:**

1. Inorganic Chemistry — Housecroft & Sharpe
2. Advanced Inorganic Chemistry — Cotton & Wilkinson
3. Basic Organometallic Chemistry: Concepts, Syntheses and Applications — B. D. Gupta, A J Elias
4. Principles of Bioinorganic Chemistry— Stephen J. Lippard & Jeremy M. Berg
5. Bioinorganic Chemistry — Asim K. Das, M. Das, A. Das & U. Das
6. Inorganic Chemistry: Principles of Structure and Reactivity; —James E. Huheey, Ellen A. Keiter, Richard L. Keiter, Okhil K. Medhi.
7. Mechanisms of Inorganic Reactions—Fred Basolo & Ralph G. Pearson
8. Electrochemical methods: fundamentals and applications —Allen J. Bard, Larry R. Faulkner

| Paper Code: CHEM-DSE-303B                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |             |           |
|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------|-----------|
| <b>Course Title:</b> Supramolecular Chemistry, Crystal Engineering and Inorganic Nanomaterials<br><b>Contact Hrs:</b> 4 Lectures per Week<br><b>Examination Duration (Hrs.):</b> Two Hours<br><b>Mode of Evaluation:</b><br><b>Continuous Assessment (CA):</b> 10 Marks<br><b>End term Examination (ETE):</b> 40 Marks<br><b>Total Credits:</b> 4<br><b>Semester:</b> III<br><b>Subject Area:</b> Applied Inorganic Chemistry<br><b>Objective:</b> To develop a comprehensive understanding of the principles, design, characterization, and applications of supramolecular chemistry, crystal engineering, and inorganic nanomaterials. |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |             |           |
| Unit                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | Contents                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | Contact Hrs |           |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | L           | T         |
| 1                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        | <b>Supramolecular Chemistry:</b> Definition, development, and scope of supramolecular chemistry; non-covalent interactions and their significance; hydrogen bonding (definition, classification, Etter's rules, and graph-set analysis); supramolecular synthon concept; $\pi$ - $\pi$ interactions (types, charge-transfer and arene-perfluoroarene interactions); role of $\pi$ -interactions in nucleic acids, proteins, and biological systems; H- and J-aggregates and their applications in optoelectronic materials; halogen bonding (definition, classification, comparison with hydrogen bonding, and unique features); polymorphism, co-crystals, and molecular salts (definition, synthesis, and significance); applications in pharmaceuticals (polymorphs and co-crystals) and optics (luminescent crystals, co-crystals, and structure-property relationships). | 20          | 7         |
| 2                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        | <b>Crystal Design, Growth, Characterization and Applications:</b> Principles of crystal design and growth; methods of crystal growth; correlation between molecular structure and crystal properties; tuning crystal properties through crystallo-chromism, polymorphism, and co-crystallization; supramolecular optical materials, including aggregation-induced emission (AIE), solid-state luminescence, and crystal engineering of fluorescent, phosphorescent, and thermally activated delayed fluorescence (TADF) materials; design and applications of TADF materials; fundamentals of electroluminescence and electroluminescent materials; multicolour emitters, hetero-structures, epitaxial growth, and applications in LEDs and OLEDs.                                                                                                                            | 20          | 7         |
| 3                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        | <b>Inorganic Nanomaterials:</b> Definition, development, and significance of nanomaterials; synthesis of metal and metal-oxide nanoparticles by reduction, solvothermal/hydrothermal, electro-spinning, micro-emulsion, combustion, microwave, gas-phase, and sol-gel methods; structure and properties, including band structure, band gap, quantum dots, nanosize effects, and quantum confinement; optical, mechanical, and electrical properties, electron transfer, and charge transport; basic characterization techniques (PXRD, SEM, TEM, AFM, and STM); applications in solar cells, LEDs, transistors, optoelectronic devices, photocatalysis, sensors, and functional coatings.                                                                                                                                                                                    | 20          | 6         |
| <b>Total Contact Hours</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | <b>60</b>   | <b>20</b> |

#### Recommended Books:

- Supramolecular Chemistry. Jonathan W. Steed and Jerry L. Atwood. Wiley 2nd Edn.
- Supramolecular Chemistry-Fundamentals and Applications. A. Katsuhiko and K. Toyoki. Springer.
- Crystal Engineering. G. R. Desiraju, J. J. Vittal and A. Ramanan. World Scientific, 1st Edn.
- Organic Crystal Engineering: Frontiers in Crystal Engineering. E. R. T. Tiekink, J. Vittal and M. Zaworotko. Wiley, 2010.
- Frontiers in Crystal Engineering. Edward R. T. Tiekink (Editor), Jagadese Vittal (Editor). Wiley, 2005.
- An Introduction to Supramolecular Chemistry. Asim K. Das, Mahua Das, CBS Publishers and Distributors Pvt Ltd. 2005.
- Introduction: Supramolecular Chemistry. Huang, F.; Anslyn, E. V. Chem. Rev. 2015, 115, 6999- 77000.
- Supramolecular materials. Amabilino, D. B.; Smith, D. K.; Steed, J. W. Chem. Soc. Rev., 2017, 46, 2404-2420.
- The Weak Hydrogen Bond: In Structural Chemistry and Biology. Desiraju, G.; Steiner, T. Oxford, IUCr Monograph on Crystallography.
- Photoluminescent organic crystals and co-crystals, Dar, A. A. and Malik, A. A Journal of Materials Chemistry C, 2024, 12 (27), 9888-9913
- C. N. R. Rao, A. Muller, A. K. Cheetham, The chemistry of nanomaterials: Synthesis, properties and applications, Wiley (2004).
- Hornyak, Dutta, Tibbals and Rao, Introduction to Nanoscience and Nanotechnology, New York, CRC press, 2008

13. J. Goldstein, D. E. Newbury, D.C. Joy, and C.E. Lym, "Scanning Electron Microscopy and X-ray Microanalysis", 2003.
14. D. Williams and B. Carter, "Transmission Electron Microscopy - A Textbook for Materials Science", Plenum Press, New York, 2nd Edition, 2009
15. AR West, Solid State chemistry and its applications, John Wiley & Sons, Ltd. 2nd Edition, 2014.
16. Y. Leng, Materials Characterization-Introduction to microscopic and spectroscopic methods. 2ndEdn. Wiley-VCH

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|----------------------------------|
| <b>Paper Code: CHEM-DSE-303C</b> |
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|-------------------------------------------|
| <b>Course Title:</b> SWAYAM MOOCs Course. |
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| To be selected in the Departmental committee meeting by choosing one of the courses offered by the SWAYAM. |
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| <b>Total Credits:</b> 4 |
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| <b>Semester:</b> III |
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**Paper Code: CHEM-DRP-304****Course Title:** Research Methodology**Contact Hrs:** 4 Hours per Week**Examination Duration (Hrs.):** Two Hours**Mode of Evaluation:****Continuous Assessment (CA):** 10 Marks**End term Examination (ETE):** 40 Marks**Total Credits:** 4**Semester:** III**Subject Area:** Research Methodology**Objective:** To acquire knowledge about the advance research methodology.

| Unit                       | Contents                                                                                                                                                                                                                                                                                                                                                                                                                         | Contact Hrs |           |
|----------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------|-----------|
|                            |                                                                                                                                                                                                                                                                                                                                                                                                                                  | L           | T         |
| 1                          | <b>Design:</b> Concept and model: theory building, testing and construction: descriptive and explanatory research: prediction, correlation and causation: deterministic and probabilistic views, pragmatization, social impact.                                                                                                                                                                                                  | 12          | 4         |
| 2                          | <b>Methodology:</b> Titrimetric method, gravimetric, chromatographic, potentiometric method of analysis, electrical (electrolysis, coulometry, polarimetry, cyclic voltametry) method of analysis, coulometry, TGA-DTA, and DSC analysis, spectrophotometric analysis, spectral techniques, principles and applications of UV, FT-IR, NMR and Mass and emission spectroscopic.                                                   | 12          | 4         |
| 3                          | <b>General Computer Application:</b> Operating system, Microsoft Office, preliminary idea about the hardware of computer, Chem draw, Origin programme, Photoshop programme, Power Point Presentation, open-source chemistry literature, Chemistry related database.                                                                                                                                                              | 12          | 4         |
| 4                          | <b>Methods and Techniques:</b> Synthetic Methodologies; thermal, photochemical, microwave-irradiation, ultra-sound mediated, room temperature, aqueous media, solvent free techniques, catalytic effects, green methods, material science; solid state synthetic methodologies, physical properties measurements, X-ray Crystallographic for characterization and molecular structure determination, SEM, TEM, BET surface area. | 12          | 4         |
| 5                          | <b>Separation techniques used in ancient India:</b> A brief overview on Rasashastra and alchemi; Extraction, distillation methods and metallurgy.<br><b>Some research works of Acharya Prafulla Chandra Ray:</b> mercuric nitrite, ammonium and aminium nitrites, gold and platinum thioether complexes.                                                                                                                         | 12          | 4         |
| <b>Total Contact Hours</b> |                                                                                                                                                                                                                                                                                                                                                                                                                                  | <b>60</b>   | <b>20</b> |

**Recommended Books:**

1. Transmission Electron Microscopy: Diffraction, Imaging, and Spectrometry by C. Barry Carter, David B. Williams, Springer International Publishing AG
2. Modern Techniques of Spectroscopy: Basics, Instrumentation, and Applications: 13 (Progress in Optical Science and Photonics) by Dheeraj Kumar Singh Manik Pradhan, Arnulf Materny, Springer International Publishing AG
3. Computer Software Applications in Chemistry by Peter C. Jurs

**Paper Code: CHEM-DRP-305**

**Course Title:** Dissertation/Research Project/Entrepreneurship

**Contact Hrs:** 16 contact hours per Week

**Examination Duration (Hrs.):**

**Mode of Evaluation:**

**Submission of Dissertation:** 60 Marks

**Presentation:** 30 Marks

**Viva-Voce:** 10 Marks

**Total Credits:** 8

**Semester:** III

**Subject Area:** Topic selection in consultation with the teacher, literature search from different reference books and using internet search, typed written-up with proper tables, structures, figures and literature to be submitted, seminar lecture on this topic to be delivered in presence of external expert and internal teachers.

**Objective:** To acquire knowledge about the advance research.

## NEP Syllabus: PG 2 Years Chemistry, Semester – IV

| Semester            | Course Type                                     | Paper Code           | Course                                         | Credit    |
|---------------------|-------------------------------------------------|----------------------|------------------------------------------------|-----------|
| IV                  | DSC                                             | <b>CHEM-DSC-401</b>  | Industrial and analytical chemistry            | 4         |
|                     | DSE                                             | <b>CHEM-DSE-402A</b> | Physical Chemistry Theory                      | 4         |
|                     |                                                 | <b>CHEM-DSE-402B</b> | Advance Physical Chemistry Theory              |           |
|                     | DSE                                             | <b>CHEM-DSE-403A</b> | Organic Chemistry Theory                       | 4         |
|                     |                                                 | <b>CHEM-DSE-403B</b> | Advance Organic Chemistry Theory               |           |
|                     |                                                 | <b>CHEM-DSE-403C</b> | SWAYAM MOOCs Course                            |           |
|                     | Dissertation/Research Project/ Entrepreneurship | <b>CHEM-DRP-404</b>  | Dissertation/Research Project/Entrepreneurship | 12        |
| <b>Total Credit</b> |                                                 |                      |                                                | <b>24</b> |

**Paper Code: CHEM-DSC-401**

**Course Title:** Industrial and Analytical Chemistry

**Contact Hrs:** 4 Lectures per Week

**Examination Duration (Hrs.):** Two Hours

**Mode of Evaluation:**

**Continuous Assessment (CA):** 10 Marks

**End term Examination (ETE):** 40 Marks

**Total Credits:** 4

**Semester:** IV

**Subject Area:** Applied Inorganic Chemistry

**Objective:** To acquire comprehensive knowledge of statistical error analysis, electrochemical analysis, experimental techniques for purification and separation, dye industries, fermentation industries, oils and oleochemical industries, and perfumery industries.

| Unit                       | Contents                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            | Contact Hrs |           |
|----------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------|-----------|
|                            |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | L           | T         |
| 1                          | <b>Statistical Error, Electrochemical Analyses:</b> Errors in quantitative analyses, types of errors, handling of systematic errors, random errors, random walk phenomenon, Normal and Gaussian distribution and its properties, standard deviation, normal distribution of mean, confidence limits of the mean, propagation of random errors, presentation of results. Method of reporting computed data. Voltammetry, Cyclic voltammetry, polarography, anodic stripping voltammetry, amperometry, coulometry, electrogravimetry. | 12          | 4         |
| 2                          | <b>Experimental Techniques of Purification and Separation:</b><br><b>Solvent Extraction:</b> principles of extraction, percentage extraction, action of ion exchange resin, ion exchange equilibria, applications. Liquid chromatography: adsorption and partition chromatography, exclusion chromatography, HPLC (principles, equipment, choice of mobile phase and detector, column efficiency, applications. Gas chromatography: Principles, instrumentation, choice of column and detector, applications.                       | 12          | 4         |
| 3                          | <b>Dyes Industries:</b> Introduction, Classification of Dyes, Colour and Contribution – Valence Bond Theory, M. O. Theory, Witt's Theory, Synthesis of Fast Red A, Naphthol Blue Black 6B, Naphthol Green B, Rosaniline, Alizarin pyronene-G<br><b>Fermentation Industries:</b> Introduction, Outline of Fermentation, Basic requirement of Fermentation, Manufacture of chloramphenicol, acetic acid, butanol, ethyl acetate, oxalic acid and citric acid.                                                                         | 12          | 4         |
| 4                          | <b>Oils and Oleochemicals Industries:</b> Introduction, Properties and classification of oils, extraction and purification of oils; Fatty acids Introduction, nomenclature and applications of fatty acids; Soap- Introduction, classification, uses and manufacturing process of soap(s), Manufacture of detergents.<br><b>Cosmetics Industries:</b> Introduction, manufacturing process of powder, cream and lotion, lipstick and nail polish, shampoo and hair dyes, tooth paste.                                                | 12          | 4         |
| 5                          | <b>Perfumery Industries:</b> Compounds used for different perfumes, Essential oils, Preparation of phenyl ethanol, Yara-Yara, $\beta$ -ionone, musk keton, musk ambrette, musk xylene, phenyl acetic acid and its esters, benzyl acetate, synthetic musk, jasmine.<br><b>Petrochemicals:</b> Petroleum refining, outline of chemicals derived from ethylene, xylene and naphthalene.                                                                                                                                                | 12          | 4         |
| <b>Total Contact Hours</b> |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | <b>60</b>   | <b>20</b> |

**Recommended Books:**

1. Stryer L., Berg J. M. and Tymoczko J. L. "Biochemistry", W. H. Freeman & Co. NY.
2. Nelson D. L. and Cox M. M., "Lehninger Principles of Biochemistry" W. H. Freeman & Company. N.
3. Mann J., "Chemical Aspects of Biosynthesis", Oxford Univ. Press.
4. Fundamentals of Analytical Chemistry— Douglas Skoog, Donald West, F. Holler, Stanley Crouch.
5. Textbook of quantitative chemical analysis— Vogel's

**Paper Code: CHEM-DSE-402A****Course Title:**Physical Chemistry Theory**Contact Hrs:** 4 Lectures per Week**Examination Duration (Hrs.):** Two Hours**Mode of Evaluation:****Continuous Assessment (CA):** 10 Marks**End term Examination (ETE):** 40 Marks**Total Credits:** 4**Semester:**IV**Subject Area:**Quantum Mechanics, Statistical Mechanics, MOFs, Nanomaterials and Data Analysis**Objective:** To acquire advance knowledge and application of quantum theory, statistical mechanics, MOFs, Nanomaterials and data analysis.

| Unit                       | Contents                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         | Contact Hrs |           |
|----------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------|-----------|
|                            |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | L           | T         |
| 1                          | <b>Theory of Many-electron Systems and their Applications:</b> The Born-Oppenheimer approximation, Hartree self-consistent field method, Koopman's theorem, Hartree-Fock method for many-electron systems. Coulomb operators, Exchange operators, Coulomb and Fermi hole, Restricted and unrestricted Hartree-Fock calculations, The Roothan equation. Correlation energy, Basis sets for electronic structure calculations. Spin-orbit interaction, The Condon-Slater rules. Introduction of density functional theory (DFT).                                                                                                                                                                                                                                                                   | 12          | 4         |
| 2                          | <b>Boltzmann, Fermi-Dirac and Bose-Einstein Statistics:</b> Canonical partition function for non-interacting distinguishable and non-identical particles. Boltzmann Statistics. Grand canonical partition function for non-interacting identical particles. Fermi-Dirac and Bose-Einstein statistics and their limiting behaviour. Ideal monoatomic gas. The translational partition function. The electric partition function. Ideal diatomic gases. The vibrational partition function. The rotational partition function of a heteronuclear molecule. The rotational partition function of a homonuclear diatomic molecule. The classical partition function. Equipartition of energy. Ideal polyatomic gas. The vibrational and the rotational partition functions. An ideal gas of photons. | 15          | 5         |
| 3                          | <b>Metal Organic Frameworks:</b> Definition, nomenclature and classification of Covalent Organic Frameworks (COFs), metal-organic frameworks (MOF's). Synthesis, physico-chemical properties and catalytic applications. Molecules encapsulation in MOF's and its applications—molecular gas cylinders (hydrogen, methane, acetylene), drug carriers (ibuprofen). Nanotechnologies based on MOF's.                                                                                                                                                                                                                                                                                                                                                                                               | 12          | 4         |
| 4                          | <b>Nano Materials:</b> Introduction and concepts of nano materials and nanoscience. Applications of nanomaterials in ancient India. Theoretical aspects nanostructured materials, 0D, 1D and 2D nanostructures, concept of quantum confinement: quantum dot, quantum wire, quantum well. Different types of nano materials, including core-shell nanostructure, nanocomposites and nanoporous materials, metal nanoparticles. Physical properties; surface, electrical and magnetical properties. Stabilization of nano particles. Carbon nano world: fullerenes, graphenes, nano-tubes. Synthesis of some nanomaterials and application of nanomaterials.                                                                                                                                       | 15          | 5         |
| 5                          | <b>Data analysis:</b> Mean and standard deviation; absolute and relative errors; linear regression; covariance and correlation coefficient.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | 6           | 2         |
| <b>Total Contact Hours</b> |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | <b>60</b>   | <b>20</b> |

**Recommended Books:**

1. Quantum Chemistry by Donald A McQuarrie
2. Quantum Mechanics second edition, by V. Devanathan
3. Quantum Chemistry fifth edition by Ira N. Levine
4. Atkins' Physical Chemistry tenth edition by Peter Atkins and Julio de Paula
5. A text book of Physical Chemistry, Quantum chemistry and Molecular Spectroscopy, volume 4 by K.L Kapoor
6. A text book of Physical Chemistry, volume 5 by K.L Kapoor
7. Introduction to Nano Science and Technologies by Anjaneyellu Yerramilli
8. The Science of Nanomaterials: Basics and Applications by Rakshit Ameta (Edited), Suresh C. Ameta (Edited).
9. Nanomaterials: An Introduction to Synthesis, Properties and Applications by Dieter Vollath
10. Statistical Mechanics by Donald A McQuarrie
11. Statistical Mechanics by RK Pathria
12. Statistical Mechanics: Principles and Selected Applications by Terrell L. Hill
13. Physical Chemistry: A Molecular Approach, Donald A. McQuarrie and John D. Simon, Viva Books
14. Physical Chemistry, P. W. Atkins, J. D. Paula and J. Keeler, Oxford University Press.
15. Statistical Mechanics, Donald A. McQuarrie

| Paper Code: CHEM-DSE-402B                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |             |           |
|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------|-----------|
| <b>Course Title:</b> Advance Physical Chemistry Theory<br><b>Contact Hrs:</b> 4 Lectures per Week<br><b>Examination Duration (Hrs.):</b> Two Hours<br><b>Mode of Evaluation:</b><br><b>Continuous Assessment (CA):</b> 10 Marks<br><b>End term Examination (ETE):</b> 40 Marks<br><b>Total Credits:</b> 4<br><b>Semester:</b> IV<br><b>Subject Area:</b> DFT, Solid State Chemistry, Molecular Simulation, Statistical Mechanics, Photochemistry<br><b>Objective:</b> To acquire advance knowledge and application of DFT, solid state chemistry, statistical mechanics, photochemistry and advance photochemistry. |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |             |           |
| Unit                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | Contents                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | Contact Hrs |           |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | L           | T         |
| 1                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | <b>Foundations of Density Functional Theory:</b> Hartree-Fock theory for many electron systems, Limitations of Hartree-Fock theory, Electron correlation and correlation energy, Configuration Interaction method, Electron density as the basic variable, Functional and Functional derivatives, Hohenberg-Kohn theorems, Kohn-Sham formulation of DFT, Kohn-Sham orbitals and orbital energies, Kohn-Sham equations, Local density approximation (LDA), Generalized gradient approximation (GGA), Perdew Burke-Ernzerhof functional (PBE), hybrid functionals (such as B3LYP), Exchange correlation, Exchange interaction, Self-interaction, Concept of potential energy surface, Janak's theorem, Transition state theory, Geometry Optimization.          | 12          | 4         |
| 2                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | <b>Advanced Solid State:</b> Specific heat of solids (Einstein & Debye models), and types of solidstate reactions, Point groups and space groups: basic concept and chemical significance, Symmetry operations in crystals, Close packing in solids: CCP, HCP, voids, and radius ratio rules, Crystal Structures: Detailed study of NaCl, CsCl, ZnS (Zinc blende & Wurtzite), Spinels, and Inverse Spinels. Advanced aspects of band theory, Density of states and Fermi surface: basic concept, p-type and n-type semiconductors, Spinel ferrites and magnetic materials, Dielectric properties of solids, Ferroelectricity, piezoelectricity, and pyroelectricity, Superconductivity. Introduction of lattice dynamics, Phonons.                            | 12          | 4         |
| 3                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | <b>Fundamentals of Molecular Dynamics Simulation:</b> Role of computer simulation in statistical mechanics, Molecular dynamics simulation, Lennard-Jones interaction, Interaction potentials and force fields, electrostatic interaction, and non-bonded interactions, Newtonian equation of motion for molecular system, Numerical integration, Verlet and velocity-Verlet algorithms, Periodic boundary conditions, Minimum image convention, Cut-off schemes and treatment of long-range interactions, Energy minimization. Nonadiabatic Molecular dynamics.                                                                                                                                                                                               | 12          | 4         |
| 4                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | <b>Ensemble Methods, Simulation Analysis, and Free Energy Calculations:</b> Simulation under different thermodynamic conditions, Molecular dynamics simulations in different ensembles. NVE, NVT, and NPT simulations. Thermostats: Berendsen, Andersen, Langevin, and NoséHoover thermostat, Barostats: basic idea and pressure coupling methods, Reduced distribution functions, Brownian motion, Potential energy functions, Hard-sphere potential, square-well potential, Lennard-Jones potential, Coulombic interaction, Calculation of thermodynamic, structural, and dynamical properties from trajectories, Mean square displacement and diffusion coefficient, Free energy calculation, Potential calculation, Entropy calculation.                  | 12          | 4         |
| 5                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | <b>Photochemistry and Advanced Photochemistry:</b> Laws of photochemistry, quantum yield, absorption and emission of radiation, Jablonski diagram, Franck-Condon principle, fluorescence, phosphorescence, internal conversion, intersystem crossing, Kasha's rule, Vavilov's rule, photochemical kinetics, quenching and Stern-Volmer equation, excimers and exciplexes, luminescence. Advanced topics include excited-state potential energy surfaces, excited-state dynamics, conical intersections, charge-transfer states, energy transfer, photoinduced electron transfer, Marcus theory, ultrafast photochemistry, photocatalysis, photoredox chemistry, semiconductor photocatalysis, solar energy conversion, and applications in materials systems. | 12          | 4         |
| <b>Total Contact Hours</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | <b>60</b>   | <b>20</b> |

**Recommended Books:**

1. Modern Quantum Mechanics — J. J. Sakurai & Jim Napolitano
2. Computational Chemistry- Errol Lewars, Kluwer Academic Publishers
3. Quantum Chemistry- Frank L Pillar
4. Quantum Chemistry- Ira N Levine
5. Density-Functional Theory of Atoms and Molecules — R. G. Parr & W. Yang

6. A Chemist's Guide to Density Functional Theory — Wolfram Koch & Max C. Holthausen
7. Understanding Molecular Simulation: From Algorithms to Applications — Daan Frenkel & Berend Smit
8. Computer Simulation of Liquids — M. P. Allen & D. J. Tildesley
9. Statistical Mechanics – Donald A McQuarrie 10. Statistical Mechanics – RK Pathria
10. Principles of Molecular Photochemistry: An Introduction — N. J. Turro, V. Ramamurthy & J. C. Scaiano
11. Modern Molecular Photochemistry of Organic Molecules — N. J. Turro, V. Ramamurthy & J. C. Scaiano
12. Photochemistry and Photophysics: Concepts, Research, Applications — Vincenzo Balzani, Paola Ceroni & Alberto Juris
13. Principles of Solid State by H.V Keer
14. Solid State Physics by A J Dekker
15. Solid State Physics second edition by J.R. Hook & H.E. Hall
16. Solid State Physics, Ashcroft and Mermin
17. Solid State Physics, R L Singhal
18. Introduction to Solid State physics, Charles Kittel

| Paper Code: CHEM-DSE-403A                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |             |           |
|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------|-----------|
| <b>Course Title:</b> Organic Chemistry Theory<br><b>Contact Hrs:</b> 4 Lectures per Week<br><b>Examination Duration (Hrs.):</b> Two Hours<br><b>Mode of Evaluation:</b><br><b>Continuous Assessment (CA):</b> 10 Marks<br><b>End term Examination (ETE):</b> 40 Marks<br><b>Total Credits:</b> 4<br><b>Semester:</b> IV<br><b>Subject Area:</b> Organic Chemistry<br><b>Objective:</b> To acquire knowledge about the asymmetric synthesis, boron, phosphorus, silicon and sulphur chemistry in organic synthesis; bond activation and functionalization in organic chemistry. |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |             |           |
| Unit                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           | Contents                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | Contact Hrs |           |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | L           | T         |
| 1                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | <b>Asymmetric Synthesis:</b> Enantio- and diastereo selective synthesis. Reactions of enolates ( $\alpha$ -substitution), Addition to C=C double bonds (electrophile induced cyclisation, iodolactonisation, Conjugate additions. Reduction of C=C double bonds, Aldol Reaction, Diels Alder Cycloaddition, Cyclopropanation, Oxidation, Epoxidation, dihydroxylation and aminohydroxylation; Rearrangement: [3,3]-Sigmatropic, (2,3)-Wittig, alkene isomerisation.                                                                                                                           | 12          | 4         |
| 2                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | <b>Boron and Phosphorus Chemistry:</b> Organoboron – Preparation and Chemistry of organo boron compounds, carboranes, hydroboration, reactions of organo boranes, unsaturated hydrocarbon synthesis, allyl boranes, boron enolates. Organo phosphorus - Chemistry of organo phosphorus compounds, Phosphorus ylides and chiral phosphines.                                                                                                                                                                                                                                                    | 12          | 4         |
| 3                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | <b>Silicon Chemistry:</b> Chemistry of organo silicon compounds, Synthetic uses of silyl ethers, silylenol ethers, TMSCN, alkene synthesis, alkynyl, vinyl, aryl, allyl and acyl silanes; Brook rearrangement, silicon Baeyer Villiger rearrangement.                                                                                                                                                                                                                                                                                                                                         | 12          | 4         |
| 4                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | <b>Sulphur Chemistry:</b> Organo sulphur- Chemistry of organo sulphur compounds, Sulphur-stabilized anions and cations, sulphonium salts, sulphonium and sulfoxonium ylides, chiral sulfoxides, umpolung.                                                                                                                                                                                                                                                                                                                                                                                     | 12          | 4         |
| 5                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | <b>Bond Activation and Functionalization:</b> Metallic or Non-metallic Approach Mechanisms of C-H bond activation with transition metals: Oxidative addition, sigma bond metathesis, electrophilic and metalloradical activation. Organic synthesis involving chelation-assisted C-H activation, ortho-C-H activation, C-H activation in heterocycles and base-assisted C-H activation. C-H, C=C and C $\equiv$ C activated annulation reactions. Important synthetic approaches via C-X (X= C, N, O, S etc.) bond activation. Role of non-metallic activation of bonds in organic synthesis. | 12          | 4         |
| <b>Total Contact Hours</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | <b>60</b>   | <b>20</b> |

**Recommended Books:**

1. Organic Synthesis - The Disconnection Approach – S. Warren
2. Designing Organic Synthesis – S. Warren
3. Tactics of Organic Synthesis - T.-L. Ho.
4. Exercise in Synthetic Organic Chemistry - C. Ghiron & R. J. Thomas.
5. Hydroboration - H. C. Brown
6. Borane Reagents - H. C. Brown, A. Pelter, K. Smith.
7. Organic Chemistry, Vol. II - I.L. Finar.
8. Relevant parts from Advanced Organic Chemistry - F.A. Carey and R.J. Sandberg; Vols. I & II.
9. Relevant parts from Comprehensive Organic Synthesis - B. M. Trost & I. Fleming.
10. Relevant parts from Comprehensive Heterocyclic Chemistry- A.R. Katritzky.
11. Advanced Organic Chemistry - J. March.
12. Mechanism and Structure in Organic Chemistry - E. S. Gould.
13. Organic Chemistry - J. B. Hendrickson, D. J. Cram & J. H. Hammond; 3<sup>rd</sup> edition.
14. Organic Chemistry – J. Clayden; N. Greeves; S. Warren & P. Wothers.
15. Organic Reaction Mechanics- A. Gallego, M. Gomer & Sierra, M.A

| Paper Code: CHEM-DSE-403B                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |             |           |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------|-----------|
| <b>Course Title:</b> Advance Organic Chemistry Theory<br><b>Contact Hrs:</b> 4 Lectures per Week<br><b>Examination Duration (Hrs.):</b> Two Hours<br><b>Mode of Evaluation:</b><br><b>Continuous Assessment (CA):</b> 10 Marks<br><b>End term Examination (ETE):</b> 40 Marks<br><b>Total Credits:</b> 4<br><b>Semester:</b> IV<br><b>Subject Area:</b> Application of Organic Chemistry<br><b>Objective:</b> To acquire knowledge about industrial application of organic chemistry; organic molecule as a organic material, drug and polymer. |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |             |           |
| Unit                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            | Contents                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | Contact Hrs |           |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | L           | T         |
| 1                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | <b>Industrial Applications of Organic Chemistry:</b> Value-added chemicals from non-renewable resources and further organic transformations. Natural gas: conversion to value-added chemicals and materials. Chemicals derived from renewable resources: Source, value-added chemicals, and products. Bulk preparation methods. Industrial chemicals derived by the Fermentation process. Surface Active Agents, detergents, and pharmaceuticals.                                                                                                                                                                                                                                                                                                                                             | 15          | 5         |
| 2                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | <b>Organic Materials (Materials Chemistry):</b> Molecular electronics: molecular materials for electronics and molecular scale electronics: Molecular properties, molecular arrangement and molecular interactions, piezoelectric and pyroelectric organic materials; molecular magnets based on transition metal complexes and organic ferromagnets, organic non-linear optical materials: photochromic organic materials and their classes; conducting polymers: polyacetylene, polypyrrole, polyaniline and polythiophene; conductive change transfer materials: TTTCNQ, metal-dithiolate systems, fullerenes. Langmuir-Blodgett films, molecular electronic logic and architectures.                                                                                                      | 15          | 5         |
| 3                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | <b>Synthesis and Uses of the following Drugs of different Pharmacological Activities:</b><br>a. Antimalerials: Quinine, Chloquine, Trimethoprim<br>b. Analgesic & Antipyretics: Paracetamol, Meperidine, methadone, Aminopyrine.<br>c. Anti-inflammatory: Aspirin, Ibuprofen, Oxyphenylbutazone, Diclophenac, Indomethacin, coxib, celecoxib.<br>d. Antitubercular and antileprotic: Ethambutol, Isoniazide & Dapsone<br>e. Anaesthetics: Lidocaine, Thiopental.<br>f. Antihistamines: Phenobarbital, Diphenylhydramine.<br>g. Tranquilizers: Diazepam, Trimeprazine<br>h. Cardiovascular: Synthesis of diltiazem, quinidine, methyl dopa, atenolol, oxyprenol<br>i. Anti-neoplastic drugs: Cancer chemotherapy, Synthesis of mechloaethamine, cyclophosphamide, Mephalan, uracils, mustards. | 15          | 5         |
| 4                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | <b>Organic and Inorganic Polymer:</b><br><b>Organic Polymer:</b> Manufacturing process, general properties, compounding and applications of SBR, Polyisoprene, Polybutadiene, Butyl rubber, Ethylene-propylene rubber, Neoprene rubber, Speciality rubbers: Silicon rubbers, Nitrile rubbers, Polyacrylic rubbers – Polyurethane rubbers – foam rubber.<br><b>Inorganic Polymers:</b> Classification of inorganic polymer, inorganic polymerisation reactions (addition, condensation and coordination polymerisation). Polysiloxanes, polysilanes, poly phosphazenes, polymeric sulfur. Synthesis, structure, properties and application of coordination polymers & organometallic polymers.                                                                                                 | 15          | 5         |
| <b>Total Contact Hours</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | <b>60</b>   | <b>20</b> |

**Recommended Books:**

1. M. A. Benvenuto, Industrial Organic Chemistry, Berlin, Boston: De Gruyter, 2017.
2. B. G. Reuben, J. S. Plotkin, H. A. Wittcoff, Industrial Organic Chemicals, Wiley, 3rd Edition, 2012
3. H. H. Szmant, Organic Building Blocks of the Chemical Industry, Wiley & Sons, 1989.
4. E. R. Riegel, J. A. Kent. Riegel's Handbook of Industrial Chemistry, 2007
5. P.J. Vander Put, Inorganic Chemistry of Materials, Plenum Press, New York, 1998.
6. M.C. Petty, M.R. Bryce and D. Bloor, Editors An Introduction to Molecular Electronics, Edward Arnold, London 1995.
7. A. Kar, Medicinal Chemistry, New Age publications.

8. Thomas Nogrady, Donald F. Weave, Medicinal Chemistry-A Molecular and Biochemical Approach, Oxford University Press.
9. Burger. Medicinal Chemistry and Drug Discovery, Vol-1, Ed. M. E. Wolff, John Wiley (1994).
10. Goodman & Gilman. Pharmacological Basis of Therapeutics, McGraw-Hill (2005).
11. S. S. Pandeya & J. R. Dimmock. Introduction to Drug Design, New Age International. (2000)
12. D. Lednicher. Strategies for Organic Drug Synthesis and Design, John Wiley (1998).
13. Graham & Patrick. Introduction to Medicinal Chemistry (3rd edn.), OUP (2005).
14. C. Tanford, Physical Chemistry of Macromolecules, Wiley, Newyork, 1961
15. V.R. Gowariker, Polymer Science, New Age International New Delhi, 1986
16. Y. Morai, Micelles: Theoretical and Applied Aspects, Plenum (1992).
17. G. Odien, Principles of Polymerization, 3rd edition (1991) John Wiley & Sons, Singapore.
18. P. Bahadur and N.V. Sastry, Principles of Polymer Science, (2002) Narosa, New Delhi.
19. F.W. Billmayer, Jr., Text Book of Polymer Science, 3rd Edition (1984), Wiley-Interscience, New Y

|                                                                                                                                                                                                                              |
|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Paper Code: CHEM-DSE-403C</b>                                                                                                                                                                                             |
| <p><b>Course Title:</b> SWAYAM MOOCs Course.</p> <p>To be selected in the Departmental committee meeting by choosing one of the courses offered by the SWAYAM.</p> <p><b>Total Credits:</b> 4</p> <p><b>Semester:</b> IV</p> |

**Paper Code: CHEM-DRP-404**

**Course Title:** Dissertation/Research Project/Entrepreneurship

**Contact Hrs:** 24 contact hours per Week

**Examination Duration (Hrs.):**

**Mode of Evaluation:**

**Submission of Dissertation:** 100 Marks

**Presentation:** 30 Marks

**Viva-Voce:** 20 Marks

**Total Credits:** 12

**Semester:** IV

**Subject Area:** Topic selection in consultation with the teacher, literature search from different reference books and using internet search, typed written-up with proper tables, structures, figures and literature to be submitted, seminar lecture on this topic to be delivered in presence of external expert and internal teachers.

**Objective:** To acquire knowledge about the advance research.

## NEP Syllabus: PG 1 Year Chemistry

|                     |                                                 |                      |                                                                           |           |
|---------------------|-------------------------------------------------|----------------------|---------------------------------------------------------------------------|-----------|
| I                   | DSC                                             | <b>CHEM-DSC-101</b>  | Physical Chemistry Theory                                                 | 4         |
|                     | DSE                                             | <b>CHEM-DSE-102A</b> | Organic Chemistry Theory                                                  | 4         |
|                     |                                                 | <b>CHEM-DSE-102B</b> | Advance Organic Chemistry Theory                                          |           |
|                     | DSE                                             | <b>CHEM-DSE-103A</b> | Inorganic Chemistry Theory                                                | 4         |
|                     |                                                 | <b>CHEM-DSE-103B</b> | Supramolecular Chemistry, Crystal Engineering and Inorganic Nanomaterials |           |
|                     |                                                 | <b>CHEM-DSE-103C</b> | SWAYAM MOOCs Course                                                       |           |
|                     | Advance Research Methodology                    | <b>CHEM-DRP-104</b>  | Advance Research Methodology                                              | 4         |
|                     | Dissertation/Research Project/ Entrepreneurship | <b>CHEM-DRP-105</b>  | Dissertation/Research Project/Entrepreneurship                            | 8         |
| <b>Total Credit</b> |                                                 |                      |                                                                           | <b>24</b> |
|                     |                                                 |                      |                                                                           |           |
| II                  | DSC                                             | <b>CHEM-DSC-201</b>  | Industrial and analytical chemistry                                       | 4         |
|                     | DSE                                             | <b>CHEM-DSE-202A</b> | Physical Chemistry Theory                                                 | 4         |
|                     |                                                 | <b>CHEM-DSE-202B</b> | Advance Physical Chemistry Theory                                         |           |
|                     | DSE                                             | <b>CHEM-DSE-203A</b> | Organic Chemistry Theory                                                  | 4         |
|                     |                                                 | <b>CHEM-DSE-203B</b> | Advance Organic Chemistry Theory                                          |           |
|                     |                                                 | <b>CHEM-DSE-203C</b> | SWAYAM MOOCs Course                                                       |           |
|                     | Dissertation/Research Project/ Entrepreneurship | <b>CHEM-DRP-204</b>  | Dissertation/Research Project/Entrepreneurship                            | 12        |
| <b>Total Credit</b> |                                                 |                      |                                                                           | <b>24</b> |

## NEP Syllabus: PG 1 Year Chemistry, Semester – I

| Semester            | Course Type                                     | Paper Code           | Course                                                                    | Credit    |
|---------------------|-------------------------------------------------|----------------------|---------------------------------------------------------------------------|-----------|
| I                   | DSC                                             | <b>CHEM-DSC-101</b>  | Physical Chemistry Theory                                                 | 4         |
|                     | DSE                                             | <b>CHEM-DSE-102A</b> | Organic Chemistry Theory                                                  | 4         |
|                     |                                                 | <b>CHEM-DSE-102B</b> | Advance Organic Chemistry Theory                                          |           |
|                     | DSE                                             | <b>CHEM-DSE-103A</b> | Inorganic Chemistry Theory                                                | 4         |
|                     |                                                 | <b>CHEM-DSE-103B</b> | Supramolecular Chemistry, Crystal Engineering and Inorganic Nanomaterials |           |
|                     |                                                 | <b>CHEM-DSE-103C</b> | SWAYAM MOOCs Course                                                       |           |
|                     | Advance Research Methodology                    | <b>CHEM-DRP-104</b>  | Advance Research Methodology                                              | 4         |
|                     | Dissertation/Research Project/ Entrepreneurship | <b>CHEM-DRP-105</b>  | Dissertation/Research Project/Entrepreneurship                            | 8         |
| <b>Total Credit</b> |                                                 |                      |                                                                           | <b>24</b> |

| Paper Code: CHEM-DSC-101                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |             |           |
|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------|-----------|
| <b>Course Title:</b> Physical Chemistry Theory<br><b>Contact Hrs:</b> 4 Lectures per Week<br><b>Examination Duration (Hrs.):</b> Two Hours<br><b>Mode of Evaluation:</b><br><b>Continuous Assessment (CA):</b> 10 Marks<br><b>End term Examination (ETE):</b> 40 Marks<br><b>Total Credits:</b> 4<br><b>Semester:</b> I<br><b>Subject Area:</b> Quantum Mechanics, Statistical Mechanics, Irreversible Thermodynamics and Solid State Chemistry<br><b>Objective:</b> To acquire knowledge of quantum theory, statistical mechanics, irreversible thermodynamics and solid state chemistry. |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |             |           |
| Unit                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       | Contents                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            | Contact Hrs |           |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | L           | T         |
| 1                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          | <b>Spin and Many Electron Wavefunctions:</b> Introduction to spin. Operator algebra for spin. Construction of matrix representation of spin operators, Eigenvalues and eigenfunctions of spin operators. Non-relativistic wavefunction for Hydrogen atom. Many-electron wavefunctions-examples with 2 and 3 electron systems, Slater determinants. Projection Operators. Parity Operator and Pauli Principle, The Pauli exclusion principle. Introduction of core, Coulomb, and exchange integrals with their properties- example of He atom.                                                                                                                                                                                       | 12          | 4         |
| 2                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          | <b>Connection between Thermodynamics and Statistical Mechanics:</b> Definition of Microstates and Macrostates. Boltzmann's definition of entropy. Formula for calculation of thermodynamic properties in terms of number of microstates. Determination of number of microstates for classical ideal gas. Connection among the properties of ideal gas, Gibbs paradox, Sackur-Tetrode equation.                                                                                                                                                                                                                                                                                                                                      | 12          | 4         |
| 3                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          | <b>Ensemble Method and its Application:</b> Definition of ensemble. A priori probability. Gibbs postulate in Statistical mechanics. Ergodic hypothesis. Prescription for studying of thermodynamic systems based on ensemble method. Preparation of equilibrium ensemble corresponding to given thermodynamic system (isolated, closed and open). Partition function. Calculation of thermodynamic properties in terms of partition function. Theory of Fluctuations. Calculation of fluctuation in energy, number of particles, density, entropy, volume, temperature etc.                                                                                                                                                         | 12          | 4         |
| 4                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          | <b>Irreversible Thermodynamics:</b> Thermodynamic criteria for Non-equilibrium states. Entropy production and Entropy balance equations. Generalized flux and forces. Stationary states. Phenomenological equations. Microscopic reversibility and Onsager equation. Applications in physico-chemical and biological phenomena. Coupled reactions.                                                                                                                                                                                                                                                                                                                                                                                  | 12          | 4         |
| 5                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          | <b>Solid State Chemistry:</b> Crystalline and amorphous structures. Reciprocal lattice concept, Brillouin zones, and their importance in electron energy levels, Bravais lattices, Miller indices, interplanar spacing, and unit cell calculations, Crystal Defects: Point defects (Schottky, Frenkel), non-stoichiometric defects (metal excess/deficiency), and F-centers, Electrical & Magnetic Properties: Band theory - Quantum mechanical aspect (Metals, Insulators, Semiconductors), Semiconductor Hall effect and Hall co-efficient, Bloch's Theorem and the Drude Model, Dielectric properties, and Magnetic properties of solids, Dia-, para-, ferro-, ferri-, and antiferromagnetism, Bragg's law and structure factor. | 12          | 4         |
| <b>Total Contact Hours</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | <b>60</b>   | <b>20</b> |

**Recommended Books:**

1. Quantum Chemistry by Donald A McQuarrie
2. Quantum Mechanics second edition, by V. Devanathan
3. Quantum Chemistry fifth edition by Ira N. Levine
4. Atkins' Physical Chemistry tenth edition by Peter Atkins and Julio de Paula
5. A text book of Physical Chemistry, Quantum chemistry and Molecular Spectroscopy, volume 4 by K.L Kapoor
6. A text book of Physical Chemistry, volume 5 by K.L Kapoor
7. Chemical Thermodynamics J. Rajaram and J.C. Kuriacose
8. Principles of Solid State by H.V Keer
9. Solid State Physics by A J Dekker
10. Solid State Physics second edition by J.R. Hook & H.E. Hall
11. Statistical Mechanics by Donald A McQuarrie
12. Statistical Mechanics by RK Pathria
13. Statistical Mechanics: Principles and Selected Applications by Terrell L. Hill

| Paper Code: CHEM-DSE-102A                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |             |           |
|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------|-----------|
| <b>Course Title:</b> Organic Chemistry Theory<br><b>Contact Hrs:</b> 4 Lectures per Week<br><b>Examination Duration (Hrs.):</b> Two Hours<br><b>Mode of Evaluation:</b><br><b>Continuous Assessment (CA):</b> 10 Marks<br><b>End term Examination (ETE):</b> 40 Marks<br><b>Total Credits:</b> 4<br><b>Semester:</b> I<br><b>Subject Area:</b> Organic Chemistry<br><b>Objective:</b> To acquire knowledge about natural product, carbohydrate chemistry, green chemistry, and photochemistry. |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |             |           |
| Unit                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           | Contents                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          | Contact Hrs |           |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | L           | T         |
| 1                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | <b>Chemistry of Natural Products – II</b><br><b>Alkaloids:</b> Introduction, general methods of isolation and structure elucidation, structure and synthesis of ephedrine, nicotine and papaverine. Structure and stereochemistry and medicinal importance of alkaloids of quinine and morphine group (cinchona and opium alkaloids).<br><b>Natural Antioxidants:</b> Chemistry of naturally occurring oxygen heterocycles, polyphenolics and other antioxidants. Use of some natural products in ayurveda as medicines in ancient India.                                                                                                                                                                                                                                                         | 15          | 5         |
| 2                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | <b>Green Chemistry:</b> Green Chemistry-Overview, Set of Principles of Green Chemistry, Green synthetic methods, Catalytic methods, Organic synthesis in aqueous media, Ionic liquid, Supercritical fluids and microwave, Solvent free organic reactions, solid phase organic synthesis.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          | 15          | 5         |
| 3                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | <b>Carbohydrate Chemistry:</b> Basic structure and type of sugars; Conformational analysis of monosaccharides (pentoses and hexoses). Protection and deprotection. <i>O</i> -glycosylation, <i>C</i> -glycosylation. Deoxysugars, amino sugars, glycal sugars and their synthetic aspects. Carbohydrates as chiral pools inorganic synthesis; Synthesis of medicinally important heterocycles derives from carbohydrates.                                                                                                                                                                                                                                                                                                                                                                         | 15          | 5         |
| 4                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | <b>Photochemistry:</b> Basic principles, Jablonski diagram, photochemistry of olefin compounds – <i>Cis/trans</i> isomerization stereomutation, photo chemistry of carbonyl compounds–Norrish Type I and Norrish Type II cleavages, photoreduction, H-atom abstraction, photocyclo addition to ketones, ethylenes, Paterno-Büchireaction, photochemistry of unsaturated ketones, esters, acids, benzoquinones, nitrite, photo fries rearrangement, Barton reaction. <i>di-pi</i> -methane rearrangement, photochemistry of arenes, Photoreaction in solid state. Method of generation and detection of radicals (ESR), radical initiators, reactivity pattern of radicals, substitution and addition reactions involving radicals, cyclisation of radicals, allylic halogenation, auto-oxidation. | 15          | 5         |
| <b>Total Contact Hours</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | <b>60</b>   | <b>20</b> |

**Recommended Books:**

- CRC Handbook of Organic Photochemistry and Photobiology. Two Volume Set-CRC Press. Axel Griesbeck, Michael Oelge möller, Francesco Ghetti.
- Introduction To Organic Photochemistry-Wiley. J. D. Coyle.
- Organic Photochemistry. Principles and Applications-Academic Press. Jacques Kagan.
- GREENE'S PROTECTIVE GROUPS IN ORGANIC SYNTHESIS, PETERG. M.WUTS, and THE ODORAW. GREENE Wiley-Inter science
- Organic Synthesis with Carbohydrates, GEERT-JANBOONS, Sheffield Academic Press, Blackwell
- The Organic Chemistry of Sugars, Edited by Daniel E. Levy Péter Fügedi, CRC

**Paper Code: CHEM-DSE-102B**

**Course Title:** Advance Organic Chemistry Theory

**Contact Hrs:** 4 Lectures per Week

**Examination Duration (Hrs.):** Two Hours

**Mode of Evaluation:**

**Continuous Assessment (CA):** 10 Marks

**End term Examination (ETE):** 40 Marks

**Total Credits:** 4

**Semester:** I

**Subject Area:** Advance Organic Chemistry

**Objective:** To acquire advanced knowledge about the most important bio-molecules and medicinal chemistry.

| Unit                       | Contents                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | Contact Hrs |           |
|----------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------|-----------|
|                            |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       | L           | T         |
| 1                          | <b>Pharmaceuticals:</b> Introduction to the clinically used drugs such as sulphonamides, antimalarials, arsenical drugs, antibiotics, the penicillin's, cephalosporin C, streptomycin, chloramphenicol, macrolide group of antibiotics, polypeptide antibiotics. General pharmacology, qualitative aspects of drug action, receptors, quantitative aspects of drug-receptor interactions, therapeutic index, various modes of administration of drugs, gram positive and negative micro-organisms, NSAID's and their mode of action. Representative antibacterial drugs, anticancer, anti-HIV drugs, their structure mode of action.                                                                                                                                                                                                                                                                                                                                                  | 15          | 5         |
| 2                          | <b>Enzymes, Coenzymes, Fermentation:</b> Enzymes- classification, mode of action, key features of active site, Chymotrypsin, Trypsin, Elastase, Michaelis- Menten model for kinetic properties of enzymes, enzymic inhibition-competitive and non-competitive. Enzymic oxidation of simple biomolecules. Cyclodextrin as Enzyme Mimics, Synzymes Cofactor, Apoenzyme, Holoenzyme, Prosthetic group, Coenzymes- catalytic role of TPP, COASH, coenzyme-I, coenzyme-II, AMP, ADP, ATP, FMN, FAD, NAD <sup>+</sup> , NADP <sup>+</sup> , NADH, NADPH, PLP, and other high energy molecules, their biogenetics, coupled reactions.                                                                                                                                                                                                                                                                                                                                                        | 15          | 5         |
| 3                          | <b>Proteins and Peptides:</b> General nature, characteristics, introduction to primary, secondary and tertiary structures. Solid Phase Peptide Synthesis: using Wang, 2-CTC, Rinkamide, Sieber amide resin. Ramachandran Plot. Separation and Purification Methods: Electrophoresis, isoelectric focusing, gel filtration, affinity chromatography, and ion exchange – choice of gel support materials (agarose, cellulose, polyacrylamide, glass beads, DEAE-cellulose, CM-cellulose etc.) HLC.<br><b>Fragmentation of Polypeptides:</b> Chemical Methods – cleavage of di-sulfide bonds; oxidation; partial acid hydrolysis; cleavages at methionine, tryptophan, tyrosine, cysteine Enzymic Methods – protein modification reactions disulphide bond cleavage, alkylation of sulphhydryl groups, modification of lysine and arginine residues. Specificity and conditions for trypsin, thrombin, chymotrypsin, thermolysin, pepsin papain etc. Determination of Peptide Sequences. | 15          | 5         |
| 4                          | <b>Nucleic Acids:</b> Human Genome project, Structure and synthesis of nucleosides and nucleotides, DN, RNA, PNA, LNA, Solid phase synthesis of DNA. DNA sequencing, replication of DNA, Transcription, Translation, mutation, genetic code, role of nucleic acid in the biosynthesis of proteins, Har Gobind Khorana Codon Chart, DNA finger printing, DNA breathing, DNA Modification and chemical carcinogenesis, P. C. reactions.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 | 15          | 5         |
| <b>Total Contact Hours</b> |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       | <b>60</b>   | <b>20</b> |

**Recommended Books:**

- 1 Stryer L., Berg J.M. and Tymoczko J. L. "Biochemistry", W. H. Freeman & Co. NY.
- 2 Nelson D. L. and Cox M. M., "Lehninger Principles of Biochemistry" W. H. Freeman & Company. NY.
- 3 Mann J., "Chemical Aspects of Biosynthesis", Oxford Univ. Press.

**Paper Code: CHEM-DSE-103A**

**Course Title:** Inorganic Chemistry Theory  
**Contact Hrs:** 4 Lectures per Week  
**Examination Duration (Hrs.):** Two Hours  
**Mode of Evaluation:**  
**Continuous Assessment (CA):** 10 Marks  
**End term Examination (ETE):** 40 Marks  
**Total Credits:** 4  
**Semester:** I  
**Subject Area:** Inorganic Chemistry  
**Objective:** To acquire comprehensive knowledge of inorganic rings, cages, and clusters; nuclear chemistry and radiochemical analysis; advanced bioinorganic chemistry; inorganic reaction mechanisms; and electrochemical analysis techniques.

| Unit                       | Contents                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         | Contact Hrs |           |
|----------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------|-----------|
|                            |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | L           | T         |
| 1                          | <b>Inorganic Rings, Cages and Clusters:</b> Stereochemistry and bonding in non-transition element compounds, Cages, clusters, rings – boranes, carboranes, metalloboranes and metallocarboranes, siloxanes, hetero-atomic rings, phosphonitrilic compounds. Metal-metal bonding (M.O. Approach), metal-metal single and multiple bonded compounds. Low nuclearity (M3, M4) and high nuclearity (M5-M10) carbonyl clusters: skeletal electron counting, Wade-Mingos-Louher rule, Jemmis rule. Application of isolobal and isoelectronic relationships, Nb and Ta clusters, Mo and W clusters. Cluster compounds in catalysis.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | 12          | 4         |
| 2                          | <b>Nuclear Chemistry &amp; Radiochemical Analysis:</b><br><b>Nuclear models:</b> Nuclear stability, terrestrial abundance and distribution, relativistic effect, electronic configuration, oxidation states, aqueous-redox- and complex-chemistry; Nuclear forces, liquid drop model, shell model, Fermi gas model; magic numbers, nuclear spin and nuclear isomerism. Nuclear reactions: Energetics, mechanism and models of nuclear reactions. Nuclear fission and nuclear fusion, fission products and fission yields. Interactions of radiation with matters, chemical effects of nuclear transmutation (elementary idea), Nuclear reactors and particle accelerators.<br><b>Radioactive Techniques:</b> Detection and measurement of radiation- GM ionization and proportional counters. Study of chemical reactions by tracer techniques, isotope exchange and kinetic isotope effect. Radiometric analysis: Isotope dilution analysis, age determination, neutron activation analysis (NAA) and their applications. Radiation hazards and safety measures.                                                                                                | 12          | 4         |
| 3                          | <b>Advanced Bioinorganic Chemistry 2:</b> Metal ion interactions with purine and pyrimidine bases, nucleosides, nucleotides and nucleic acids, DNA and RNA, metal ions in genetic information transfer.<br><b>Redox enzymes:</b> Catalase, peroxidase, super oxide dismutase (SOD), cytochrome P-450, nitric oxide synthases (NOS), ascorbate oxidase, aldehyde oxidase; molybdo enzymes: xanthenes oxidase, nitrate reductase, sulphite oxidase including some model study.<br><b>Vitamins and coenzymes:</b> Vitamin B6 and vitamin B12 coenzymes, model systems;<br><b>Supramolecular chemistry:</b> Metal in medicine: anticancer drugs.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | 12          | 4         |
| 4                          | <b>Inorganic Reaction Mechanism:</b> Mechanism of substitution reactions, solvent exchange, aquation, anation, base hydrolysis, acid catalyzed aquation, pseudo-substitution. Energy profile diagram of ligand substitution reactions- associative (A), dissociative (D), interchange (I) etc. type pathways, relation between intimate and stoichiometric mechanisms of ligand substitution, some important rate laws, activation parameters ( $\Delta S^\ddagger$ , $\Delta H^\ddagger$ , $\Delta V^\ddagger$ ), mechanism of isomerization reaction-linkage isomerism, cis-trans isomerism, intramolecular and intermolecular racemization, Ray-Dutt and Bailar twist mechanisms, substitution in octahedral complexes- the Eigen-Wilkins mechanism, the Fuoss-Eigen equation, linear free energy relation (LFER) etc.<br><b>Mechanism of electron transfer reactions:</b> General characteristics and classification of redox reactions, self-exchange reactions. Frank-Condon principle (non-mathematical treatment). Outer sphere and Inner sphere reactions, applications of Marcus expression (simple form), and redox catalyzed substitution reactions. | 12          | 4         |
| 5                          | <b>Electrochemical analyses:</b> Introduction to electrochemical methods, electrochemical cells, diffusion controlled limiting current, voltage scanning polarography, shape and interpretation of polarographic wave, current-voltage relationship during electrolysis. Principles and applications of Voltammetry, cyclic voltammetry, polarography, anodic stripping voltammetry, amperometry, coulometry, electro-gravimetry. Spectro-electrochemistry, Hyphenated techniques; Fuel cells.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | 12          | 4         |
| <b>Total Contact Hours</b> |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | <b>60</b>   | <b>20</b> |

**Recommended Books:**

1. Inorganic Chemistry — Housecroft & Sharpe
2. Advanced Inorganic Chemistry — Cotton & Wilkinson
3. Basic Organometallic Chemistry: Concepts, Syntheses and Applications — B. D. Gupta, A J Elias
4. Principles of Bioinorganic Chemistry— Stephen J. Lippard & Jeremy M. Berg
5. Bioinorganic Chemistry — Asim K. Das, M. Das, A. Das & U. Das
6. Inorganic Chemistry: Principles of Structure and Reactivity; —James E. Huheey, Ellen A. Keiter, Richard L. Keiter, Okhil K. Medhi.
7. Mechanisms of Inorganic Reactions—Fred Basolo & Ralph G. Pearson
8. Electrochemical methods: fundamentals and applications —Allen J. Bard, Larry R. Faulkner

| Paper Code: CHEM-DSE-103B                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |             |           |
|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------|-----------|
| <b>Course Title:</b> Supramolecular Chemistry, Crystal Engineering and Inorganic Nanomaterials<br><b>Contact Hrs:</b> 4 Lectures per Week<br><b>Examination Duration (Hrs.):</b> Two Hours<br><b>Mode of Evaluation:</b><br><b>Continuous Assessment (CA):</b> 10 Marks<br><b>End term Examination (ETE):</b> 40 Marks<br><b>Total Credits:</b> 4<br><b>Semester:</b> I<br><b>Subject Area:</b> Applied Inorganic Chemistry<br><b>Objective:</b> To develop a comprehensive understanding of the principles, design, characterization, and applications of supramolecular chemistry, crystal engineering, and inorganic nanomaterials. |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |             |           |
| Unit                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | Contents                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | Contact Hrs |           |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | L           | T         |
| 1                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | <b>Supramolecular Chemistry:</b> Definition, development, and scope of supramolecular chemistry; non-covalent interactions and their significance; hydrogen bonding (definition, classification, Etter's rules, and graph-set analysis); supramolecular synthon concept; $\pi$ - $\pi$ interactions (types, charge-transfer and arene-perfluoroarene interactions); role of $\pi$ -interactions in nucleic acids, proteins, and biological systems; H- and J-aggregates and their applications in optoelectronic materials; halogen bonding (definition, classification, comparison with hydrogen bonding, and unique features); polymorphism, co-crystals, and molecular salts (definition, synthesis, and significance); applications in pharmaceuticals (polymorphs and co-crystals) and optics (luminescent crystals, co-crystals, and structure-property relationships). | 20          | 7         |
| 2                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | <b>Crystal Design, Growth, Characterization and Applications:</b> Principles of crystal design and growth; methods of crystal growth; correlation between molecular structure and crystal properties; tuning crystal properties through crystallo-chromism, polymorphism, and co-crystallization; supramolecular optical materials, including aggregation-induced emission (AIE), solid-state luminescence, and crystal engineering of fluorescent, phosphorescent, and thermally activated delayed fluorescence (TADF) materials; design and applications of TADF materials; fundamentals of electroluminescence and electroluminescent materials; multicolour emitters, hetero-structures, epitaxial growth, and applications in LEDs and OLEDs.                                                                                                                            | 20          | 7         |
| 3                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | <b>Inorganic Nanomaterials:</b> Definition, development, and significance of nanomaterials; synthesis of metal and metal-oxide nanoparticles by reduction, solvothermal/hydrothermal, electro-spinning, micro-emulsion, combustion, microwave, gas-phase, and sol-gel methods; structure and properties, including band structure, band gap, quantum dots, nanosize effects, and quantum confinement; optical, mechanical, and electrical properties, electron transfer, and charge transport; basic characterization techniques (PXRD, SEM, TEM, AFM, and STM); applications in solar cells, LEDs, transistors, optoelectronic devices, photocatalysis, sensors, and functional coatings.                                                                                                                                                                                    | 20          | 6         |
| <b>Total Contact Hours</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | <b>60</b>   | <b>20</b> |

#### Recommended Books:

- Supramolecular Chemistry. Jonathan W. Steed and Jerry L. Atwood. Wiley 2nd Edn.
- Supramolecular Chemistry-Fundamentals and Applications. A. Katsuhiko and K. Toyoki. Springer.
- Crystal Engineering. G. R. Desiraju, J. J. Vittal and A. Ramanan. World Scientific, 1st Edn.
- Organic Crystal Engineering: Frontiers in Crystal Engineering. E. R. T. Tiekink, J. Vittal and M. Zaworotko. Wiley, 2010.
- Frontiers in Crystal Engineering. Edward R. T. Tiekink (Editor), Jagadese Vittal (Editor). Wiley, 2005.
- An Introduction to Supramolecular Chemistry. Asim K. Das, Mahua Das, CBS Publishers and Distributors Pvt Ltd. 2005.
- Introduction: Supramolecular Chemistry. Huang, F.; Anslyn, E. V. Chem. Rev. 2015, 115, 6999- 77000.
- Supramolecular materials. Amabilino, D. B.; Smith, D. K.; Steed, J. W. Chem. Soc. Rev., 2017, 46, 2404-2420.
- The Weak Hydrogen Bond: In Structural Chemistry and Biology. Desiraju, G.; Steiner, T. Oxford, IUCr Monograph on Crystallography.
- Photoluminescent organic crystals and co-crystals, Dar, A. A. and Malik, A. A Journal of Materials Chemistry C, 2024, 12 (27), 9888-9913
- C. N. R. Rao, A. Muller, A. K. Cheetham, The chemistry of nanomaterials: Synthesis, properties and applications, Wiley (2004).

12. Hornyak, Dutta, Tibbals and Rao, Introduction to Nanoscience and Nanotechnology, New York, CRC press, 2008
13. J. Goldstein, D. E. Newbury, D.C. Joy, and C.E. Lym, "Scanning Electron Microscopy and X-ray Microanalysis", 2003.
14. D. Williams and B. Carter, "Transmission Electron Microscopy - A Textbook for Materials Science", Plenum Press, New York, 2nd Edition, 2009.
15. AR West, Solid State chemistry and its applications, John Wiley & Sons, Ltd. 2nd Edition, 2014.
16. Y. Leng, Materials Characterization-Introduction to microscopic and spectroscopic methods. 2ndEdn. Wiley-VCH

|                                                                                                                                                                                                                      |
|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Paper Code: CHEM-DSE-103C</b>                                                                                                                                                                                     |
| <b>Course Title:</b> SWAYAM MOOCs Course.<br><br>To be selected in the Departmental committee meeting by choosing one of the courses offered by the SWAYAM.<br><br><b>Total Credits:</b> 4<br><br><b>Semester:</b> I |

| Paper Code: CHEM-DRP-104                                                                                                                                                                                                                                                                                                                                                                                                                       |                                                                                                                                                                                                                                                                                                                                                                                                                                  |             |           |
|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------|-----------|
| <b>Course Title:</b> Research Methodology<br><b>Contact Hrs:</b> 4 Hours per Week<br><b>Examination Duration (Hrs.):</b> Two Hours<br><b>Mode of Evaluation:</b><br><b>Continuous Assessment (CA):</b> 10 Marks<br><b>End term Examination (ETE):</b> 40 Marks<br><b>Total Credits:</b> 4<br><b>Semester:</b> I<br><b>Subject Area:</b> Research Methodology<br><b>Objective:</b> To acquire knowledge about the advance research methodology. |                                                                                                                                                                                                                                                                                                                                                                                                                                  |             |           |
| Unit                                                                                                                                                                                                                                                                                                                                                                                                                                           | Contents                                                                                                                                                                                                                                                                                                                                                                                                                         | Contact Hrs |           |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                |                                                                                                                                                                                                                                                                                                                                                                                                                                  | L           | T         |
| 1                                                                                                                                                                                                                                                                                                                                                                                                                                              | <b>Design:</b> Concept and model: theory building, testing and construction: descriptive and explanatory research: prediction, correlation and causation: deterministic and probabilistic views, pragmatization, social impact.                                                                                                                                                                                                  | 12          | 4         |
| 2                                                                                                                                                                                                                                                                                                                                                                                                                                              | <b>Methodology:</b> Titrimetric method, gravimetric, chromatographic, potentiometric method of analysis, electrical (electrolysis, coulometry, polarimetry, cyclic voltametry) method of analysis, coulometry, TGA-DTA, and DSC analysis, spectrophotometric analysis, spectral techniques, principles and applications of UV, FT-IR, NMR and Mass and emission spectroscopic.                                                   | 12          | 4         |
| 3                                                                                                                                                                                                                                                                                                                                                                                                                                              | <b>General Computer Application:</b> Operating system, Microsoft Office, preliminary idea about the hardware of computer, Chem draw, Origin programme, Photoshop programme, Power Point Presentation, open-source chemistry literature, Chemistry related database.                                                                                                                                                              | 12          | 4         |
| 4                                                                                                                                                                                                                                                                                                                                                                                                                                              | <b>Methods and Techniques:</b> Synthetic Methodologies; thermal, photochemical, microwave-irradiation, ultra-sound mediated, room temperature, aqueous media, solvent free techniques, catalytic effects, green methods, material science; solid state synthetic methodologies, physical properties measurements, X-ray Crystallographic for characterization and molecular structure determination, SEM, TEM, BET surface area. | 12          | 4         |
| 5                                                                                                                                                                                                                                                                                                                                                                                                                                              | <b>Separation techniques used in ancient India:</b> A brief overview on Rasashastra and alchemi; Extraction, distillation methods and metallurgy.<br><b>Some research works of Acharya Prafulla Chandra Ray:</b> mercuric nitrite, ammonium and aminium nitrites, gold and platinum thioether complexes.                                                                                                                         | 12          | 4         |
| <b>Total Contact Hours</b>                                                                                                                                                                                                                                                                                                                                                                                                                     |                                                                                                                                                                                                                                                                                                                                                                                                                                  | <b>60</b>   | <b>20</b> |

**Recommended Books:**

1. Transmission Electron Microscopy: Diffraction, Imaging, and Spectrometry by C. Barry Carter, David B. Williams, Springer International Publishing AG
2. Modern Techniques of Spectroscopy: Basics, Instrumentation, and Applications: 13 (Progress in Optical Science and Photonics) by Dheeraj Kumar Singh Manik Pradhan, Arnulf Materny, Springer International Publishing AG
3. Computer Software Applications in Chemistry by Peter C. Jurs

**Paper Code: CHEM-DRP-105**

**Course Title:** Dissertation/Research Project/Entrepreneurship

**Contact Hrs:** 16 contact hours per Week

**Examination Duration (Hrs.):**

**Mode of Evaluation:**

**Submission of Dissertation:** 60 Marks

**Presentation:** 30 Marks

**Viva-Voce:** 10 Marks

**Total Credits:** 8

**Semester:** I

**Subject Area:** Topic selection in consultation with the teacher, literature search from different reference books and using internet search, typed written-up with proper tables, structures, figures and literature to be submitted, seminar lecture on this topic to be delivered in presence of external expert and internal teachers.

**Objective:** To acquire knowledge about the advance research.

## NEP Syllabus: PG 1 Year Chemistry, Semester – II

| Semester            | Course Type                                     | Paper Code           | Course                                         | Credit    |
|---------------------|-------------------------------------------------|----------------------|------------------------------------------------|-----------|
| II                  | DSC                                             | <b>CHEM-DSC-201</b>  | Industrial and analytical chemistry            | 4         |
|                     | DSE                                             | <b>CHEM-DSE-202A</b> | Physical Chemistry Theory                      | 4         |
|                     |                                                 | <b>CHEM-DSE-202B</b> | Advance Physical Chemistry Theory              |           |
|                     | DSE                                             | <b>CHEM-DSE-203A</b> | Organic Chemistry Theory                       | 4         |
|                     |                                                 | <b>CHEM-DSE-203B</b> | Advance Organic Chemistry Theory               |           |
|                     |                                                 | <b>CHEM-DSE-203C</b> | SWAYAM MOOCs Course                            |           |
|                     | Dissertation/Research Project/ Entrepreneurship | <b>CHEM-DRP-204</b>  | Dissertation/Research Project/Entrepreneurship | 12        |
| <b>Total Credit</b> |                                                 |                      |                                                | <b>24</b> |

**Paper Code: CHEM-DSC-201**

**Course Title:** Industrial and Analytical Chemistry

**Contact Hrs:** 4 Lectures per Week

**Examination Duration (Hrs.):** Two Hours

**Mode of Evaluation:**

**Continuous Assessment (CA):** 10 Marks

**End term Examination (ETE):** 40 Marks

**Total Credits:** 4

**Semester:** II

**Subject Area:** Applied Inorganic Chemistry

**Objective:** To acquire comprehensive knowledge of statistical error analysis, electrochemical analysis, experimental techniques for purification and separation, dye industries, fermentation industries, oils and oleochemical industries, and perfumery industries.

| Unit                       | Contents                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            | Contact Hrs |           |
|----------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------|-----------|
|                            |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | L           | T         |
| 1                          | <b>Statistical Error, Electrochemical Analyses:</b> Errors in quantitative analyses, types of errors, handling of systematic errors, random errors, random walk phenomenon, Normal and Gaussian distribution and its properties, standard deviation, normal distribution of mean, confidence limits of the mean, propagation of random errors, presentation of results. Method of reporting computed data. Voltammetry, Cyclic voltammetry, polarography, anodic stripping voltammetry, amperometry, coulometry, electrogravimetry. | 12          | 4         |
| 2                          | <b>Experimental Techniques of Purification and Separation:</b><br><b>Solvent Extraction:</b> principles of extraction, percentage extraction, action of ion exchange resin, ion exchange equilibria, applications. Liquid chromatography: adsorption and partition chromatography, exclusion chromatography, HPLC (principles, equipment, choice of mobile phase and detector, column efficiency, applications. Gas chromatography: Principles, instrumentation, choice of column and detector, applications.                       | 12          | 4         |
| 3                          | <b>Dyes Industries:</b> Introduction, Classification of Dyes, Colour and Contribution – Valence Bond Theory, M. O. Theory, Witt's Theory, Synthesis of Fast Red A, Naphthol Blue Black 6B, Naphthol Green B, Rosaniline, Alizarin pyronene-G<br><b>Fermentation Industries:</b> Introduction, Outline of Fermentation, Basic requirement of Fermentation, Manufacture of chloramphenicol, acetic acid, butanol, ethyl acetate, oxalic acid and citric acid.                                                                         | 12          | 4         |
| 4                          | <b>Oils and Oleochemicals Industries:</b> Introduction, Properties and classification of oils, extraction and purification of oils; Fatty acids Introduction, nomenclature and applications of fatty acids; Soap- Introduction, classification, uses and manufacturing process of soap(s), Manufacture of detergents.<br><b>Cosmetics Industries:</b> Introduction, manufacturing process of powder, cream and lotion, lipstick and nail polish, shampoo and hair dyes, tooth paste.                                                | 12          | 4         |
| 5                          | <b>Perfumery Industries:</b> Compounds used for different perfumes, Essential oils, Preparation of phenyl ethanol, Yara-Yara, $\beta$ -ionone, musk keton, musk ambrette, musk xylene, phenyl acetic acid and its esters, benzyl acetate, synthetic musk, jasmine.<br><b>Petrochemicals:</b> Petroleum refining, outline of chemicals derived from ethylene, xylene and naphthalene.                                                                                                                                                | 12          | 4         |
| <b>Total Contact Hours</b> |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | <b>60</b>   | <b>20</b> |

**Recommended Books:**

1. Stryer L., Berg J. M. and Tymoczko J. L. "Biochemistry", W. H. Freeman & Co. N.Y.
2. Nelson D. L. and Cox M. M., "Lehninger Principles of Biochemistry" W. H. Freeman & Company. N.
3. Mann J., "Chemical Aspects of Biosynthesis", Oxford Univ. Press.
4. Fundamentals of Analytical Chemistry— Douglas Skoog, Donald West, F. Holler, Stanley Crouch.
5. Textbook of quantitative chemical analysis— Vogel's

## Paper Code: CHEM-DSE-202A

**Course Title:**Physical Chemistry Theory  
**Contact Hrs:** 4 Lectures per Week  
**Examination Duration (Hrs.):** Two Hours  
**Mode of Evaluation:**  
**Continuous Assessment (CA):** 10 Marks  
**End term Examination (ETE):** 40 Marks  
**Total Credits:** 4  
**Semester:** II  
**Subject Area:**Quantum Mechanics, Statistical Mechanics, MOFs, Nanomaterials and Data Analysis  
**Objective:** Toacquire advance knowledge and application of quantum theory, statistical mechanics, MOFs, Nanomaterials and data analysis.

| Unit                       | Contents                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         | Contact Hrs |           |
|----------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------|-----------|
|                            |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | L           | T         |
| 1                          | <b>Theory of Many-electron Systems and their Applications:</b> The Born-Oppenheimer approximation, Hartree self-consistent field method, Koopman's theorem, Hartree-Fock method for many-electron systems. Coulomb operators, Exchange operators, Coulomb and Fermi hole, Restricted and unrestricted Hartree-Fock calculations, The Roothan equation. Correlation energy, Basis sets for electronic structure calculations. Spin-orbit interaction, The Condon-Slater rules.Introduction of density functional theory (DFT).                                                                                                                                                                                                                                                                    | 12          | 4         |
| 2                          | <b>Boltzmann, Fermi-Dirac and Bose-Einstein Statistics:</b> Canonical partition function for non-interacting distinguishable and non-identical particles. Boltzmann Statistics. Grand canonical partition function for non-interacting identical particles. Fermi-Dirac and Bose-Einstein statistics and their limiting behaviour. Ideal monoatomic gas. The translational partition function. The electric partition function. Ideal diatomic gases. The vibrational partition function. The rotational partition function of a heteronuclear molecule. The rotational partition function of a homonuclear diatomic molecule. The classical partition function. Equipartition of energy. Ideal polyatomic gas. The vibrational and the rotational partition functions. An ideal gas of photons. | 15          | 5         |
| 3                          | <b>Metal Organic Frameworks:</b> Definition, nomenclature and classification of Covalent Organic Frameworks (COFs), metal-organic frameworks (MOF's). Synthesis, physico-chemical properties and catalytic applications. Molecules encapsulation in MOF's and Its applications–molecular gas cylinders (hydrogen, methane, acetylene), drug carriers (ibuprofen). Nanotechnologies based on MOF's.                                                                                                                                                                                                                                                                                                                                                                                               | 12          | 4         |
| 4                          | <b>Nano Materials:</b> Introduction and concepts of nano materials and nanoscience. Applications of nanomaterials in ancient India. Theoretical aspects nanostructured materials, 0D, 1D and 2D nanostructures, concept of quantum confinement: quantum dot, quantum wire, quantum well. Different types of nano materials, including core-shell nanostructure, nanocomposites and nanoporous materials, metal nanoparticles. Physical properties; surface, electrical and magnetical properties. Stabilization of nano particles. Carbon nano world: fullerenes, graphenes, nano-tubes. Synthesis of some nanomaterials and application of nanomaterials. Applications of nanomaterials in ancient India.                                                                                       | 15          | 5         |
| 5                          | <b>Data analysis:</b> Mean and standard deviation; absolute and relative errors; linear regression; covariance and correlation coefficient.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | 6           | 2         |
| <b>Total Contact Hours</b> |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | <b>60</b>   | <b>20</b> |

### Recommended Books:

1. Quantum Chemistry by Donald A McQuarrie
2. Quantum Mechanics second edition, by V. Devanathan
3. Quantum Chemistry fifth edition by Ira N. Levine
4. Atkins'Physical Chemistry tenth edition by Peter Atkins and Julio de Paula
5. A text book of Physical Chemistry, Quantum chemistry and Molecular Spectroscopy, volume 4 by K.L Kapoor
6. A text book of Physical Chemistry, volume 5 by K.L Kapoor
7. Introduction to Nano Science and Technologies by Anjaneyellu Yerramilli
8. The Science of Nanomaterials: Basics and Applications by Rakshit Ameta (Edited), Suresh C. Ameta (Edited).
9. Nanomaterials: An Introduction to Synthesis, Properties and Applications by Dieter Vollath
10. Statistical Mechanics by Donald A McQuarrie
11. Statistical Mechanics by RK Pathria
12. Statistical Mechanics: Principles and Selected Applications by Terrell L. Hill
13. Physical Chemistry: A Molecular Approach, Donald A. McQuarrie and John D. Simon, Viva Books
14. Physical Chemistry, P. W. Atkins, J. D. Paula and J. Keeler, Oxford University Press.
15. Statistical Mechanics, Donald A. McQuarrie

**Paper Code: CHEM-DSE-202B****Course Title:** Advance Physical Chemistry Theory**Contact Hrs:** 4 Lectures per Week**Examination Duration (Hrs.):** Two Hours**Mode of Evaluation:****Continuous Assessment (CA):** 10 Marks**End term Examination (ETE):** 40 Marks**Total Credits:** 4**Semester:** II**Subject Area:** DFT, Solid State Chemistry, Molecular Simulation, Statistical Mechanics, Photochemistry**Objective:** To acquire advance knowledge and application of DFT, solid state chemistry, statistical mechanics, photochemistry and advance photochemistry.

| Unit                       | Contents                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | Contact Hrs |           |
|----------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------|-----------|
|                            |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | L           | T         |
| 1                          | <b>Foundations of Density Functional Theory:</b> Hartree-Fock theory for many electron systems, Limitations of Hartree-Fock theory, Electron correlation and correlation energy, Configuration Interaction method, Electron density as the basic variable, Functional and Functional derivatives, Hohenberg-Kohn theorems, Kohn-Sham formulation of DFT, Kohn-Sham orbitals and orbital energies, Kohn-Sham equations, Local density approximation (LDA), Generalized gradient approximation (GGA), Perdew Burke-Ernzerhof functional (PBE), hybrid functionals (such as B3LYP), Exchange correlation, Exchange interaction, Self-interaction, Concept of potential energy surface, Janak's theorem, Transition state theory, Geometry Optimization.          | 12          | 4         |
| 2                          | <b>Advanced Solid State:</b> Specific heat of solids (Einstein & Debye models), and types of solidstate reactions, Point groups and space groups: basic concept and chemical significance, Symmetry operations in crystals, Close packing in solids: CCP, HCP, voids, and radius ratio rules, Crystal Structures: Detailed study of NaCl, CsCl, ZnS (Zinc blende & Wurtzite), Spinel, and Inverse Spinel. Advanced aspects of band theory, Density of states and Fermi surface: basic concept, p-type and n-type semiconductors, Spinel ferrites and magnetic materials, Dielectric properties of solids, Ferroelectricity, piezoelectricity, and pyroelectricity, Superconductivity. Introduction of lattice dynamics, Phonons.                              | 12          | 4         |
| 3                          | <b>Fundamentals of Molecular Dynamics Simulation:</b> Role of computer simulation in statistical mechanics, Molecular dynamics simulation, Lennard-Jones interaction, Interaction potentials and force fields, electrostatic interaction, and non-bonded interactions, Newtonian equation of motion for molecular system, Numerical integration, Verlet and velocity-Verlet algorithms, Periodic boundary conditions, Minimum image convention, Cut-off schemes and treatment of long-range interactions, Energy minimization. Nonadiabatic Molecular dynamics.                                                                                                                                                                                               | 12          | 4         |
| 4                          | <b>Ensemble Methods, Simulation Analysis, and Free Energy Calculations:</b> Simulation under different thermodynamic conditions, Molecular dynamics simulations in different ensembles. NVE, NVT, and NPT simulations. Thermostats: Berendsen, Andersen, Langevin, and NoséHoover thermostat, Barostats: basic idea and pressure coupling methods, Reduced distribution functions, Brownian motion, Potential energy functions, Hard-sphere potential, square-well potential, Lennard-Jones potential, Coulombic interaction, Calculation of thermodynamic, structural, and dynamical properties from trajectories, Mean square displacement and diffusion coefficient, Free energy calculation, Potential calculation, Entropy calculation.                  | 12          | 4         |
| 5                          | <b>Photochemistry and Advanced Photochemistry:</b> Laws of photochemistry, quantum yield, absorption and emission of radiation, Jablonski diagram, Franck-Condon principle, fluorescence, phosphorescence, internal conversion, intersystem crossing, Kasha's rule, Vavilov's rule, photochemical kinetics, quenching and Stern-Volmer equation, excimers and exciplexes, luminescence. Advanced topics include excited-state potential energy surfaces, excited-state dynamics, conical intersections, charge-transfer states, energy transfer, photoinduced electron transfer, Marcus theory, ultrafast photochemistry, photocatalysis, photoredox chemistry, semiconductor photocatalysis, solar energy conversion, and applications in materials systems. | 12          | 4         |
| <b>Total Contact Hours</b> |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | <b>60</b>   | <b>20</b> |

**Recommended Books:**

1. Modern Quantum Mechanics — J. J. Sakurai & Jim Napolitano
2. Computational Chemistry- Errol Lewars, Kluwer Academic Publishers
3. Quantum Chemistry- Frank L Pillar
4. Quantum Chemistry- Ira N Levine
5. Density-Functional Theory of Atoms and Molecules — R. G. Parr & W. Yang

6. A Chemist's Guide to Density Functional Theory — Wolfram Koch & Max C. Holthausen
7. Understanding Molecular Simulation: From Algorithms to Applications — Daan Frenkel & Berend Smit
8. Computer Simulation of Liquids — M. P. Allen & D. J. Tildesley
9. Statistical Mechanics – Donald A McQuarrie 10. Statistical Mechanics – RK Pathria
10. Principles of Molecular Photochemistry: An Introduction — N. J. Turro, V. Ramamurthy & J. C. Scaiano
11. Modern Molecular Photochemistry of Organic Molecules — N. J. Turro, V. Ramamurthy & J. C. Scaiano
12. Photochemistry and Photophysics: Concepts, Research, Applications — Vincenzo Balzani, Paola Ceroni & Alberto Juris
13. Principles of Solid State by H.V Keer
14. Solid State Physics by A J Dekker
15. Solid State Physics second edition by J.R. Hook & H.E. Hall
16. Solid State Physics, Ashcroft and Mermin
17. Solid State Physics, R L Singhal
18. Introduction to Solid State physics, Charles Kittel

| Paper Code: CHEM-DSE-203A                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |             |           |
|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------|-----------|
| <b>Course Title:</b> Organic Chemistry Theory<br><b>Contact Hrs:</b> 4 Lectures per Week<br><b>Examination Duration (Hrs.):</b> Two Hours<br><b>Mode of Evaluation:</b><br><b>Continuous Assessment (CA):</b> 10 Marks<br><b>End term Examination (ETE):</b> 40 Marks<br><b>Total Credits:</b> 4<br><b>Semester:</b> II<br><b>Subject Area:</b> Organic Chemistry<br><b>Objective:</b> To acquire knowledge about the asymmetric synthesis, boron, phosphorus, silicon and sulphur chemistry in organic synthesis; bond activation and functionalization in organic chemistry. |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |             |           |
| Unit                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           | Contents                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | Contact Hrs |           |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | L           | T         |
| 1                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | <b>Asymmetric Synthesis:</b> Enantio- and diastereo selective synthesis. Reactions of enolates ( $\alpha$ -substitution), Addition to C=C double bonds (electrophile induced cyclisation, iodolactonisation, Conjugate additions. Reduction of C=C double bonds, Aldol Reaction, Diels Alder Cycloaddition, Cyclopropanation, Oxidation, Epoxidation, dihydroxylation and aminohydroxylation; Rearrangement: [3,3]-Sigmatropic, (2,3)-Wittig, alkene isomerisation.                                                                                                                           | 12          | 4         |
| 2                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | <b>Boron and Phosphorus Chemistry:</b> Organoboron – Preparation and Chemistry of organo boron compounds, carboranes, hydroboration, reactions of organo boranes, unsaturated hydrocarbon synthesis, allyl boranes, boron enolates. Organo phosphorus - Chemistry of organo phosphorus compounds, Phosphorus ylides and chiral phosphines.                                                                                                                                                                                                                                                    | 12          | 4         |
| 3                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | <b>Silicon Chemistry:</b> Chemistry of organo silicon compounds, Synthetic uses of silyl ethers, silylenol ethers, TMSiCl, alkene synthesis, alkynyl, vinyl, aryl, allyl and acyl silanes; Brook rearrangement, silicon Baeyer Villiger rearrangement.                                                                                                                                                                                                                                                                                                                                        | 12          | 4         |
| 4                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | <b>Sulphur Chemistry:</b> Organo sulphur- Chemistry of organo sulphur compounds, Sulphur-stabilized anions and cations, sulphonium salts, sulphonium and sulfoxonium ylides, chiral sulfoxides, umpolung.                                                                                                                                                                                                                                                                                                                                                                                     | 12          | 4         |
| 5                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | <b>Bond Activation and Functionalization:</b> Metallic or Non-metallic Approach Mechanisms of C-H bond activation with transition metals: Oxidative addition, sigma bond metathesis, electrophilic and metalloradical activation. Organic synthesis involving chelation-assisted C-H activation, ortho-C-H activation, C-H activation in heterocycles and base-assisted C-H activation. C-H, C=C and C $\equiv$ C activated annulation reactions. Important synthetic approaches via C-X (X= C, N, O, S etc.) bond activation. Role of non-metallic activation of bonds in organic synthesis. | 12          | 4         |
| <b>Total Contact Hours</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | <b>60</b>   | <b>20</b> |

**Recommended Books:**

1. Organic Synthesis - The Disconnection Approach – S. Warren
2. Designing Organic Synthesis – S. Warren
3. Tactics of Organic Synthesis - T.-L. Ho.
4. Exercise in Synthetic Organic Chemistry - C. Ghiron & R. J. Thomas.
5. Hydroboration - H. C. Brown
6. Borane Reagents - H. C. Brown, A. Pelter, K. Smith.
7. Organic Chemistry, Vol. II - I.L. Finar.
8. Relevant parts from Advanced Organic Chemistry - F.A. Carey and R.J. Sandberg; Vols. I & II.
9. Relevant parts from Comprehensive Organic Synthesis - B. M. Trost & I. Fleming.
10. Relevant parts from Comprehensive Heterocyclic Chemistry- A.R. Katritzky.
11. Advanced Organic Chemistry - J. March.
12. Mechanism and Structure in Organic Chemistry - E. S. Gould.
13. Organic Chemistry - J. B. Hendrickson, D. J. Cram & J. H. Hammond; 3<sup>rd</sup> edition.
14. Organic Chemistry – J. Clayden; N. Greeves; S. Warren & P. Wothers.
15. Organic Reaction Mechanics- A. Gallego, M. Gomer & Sierra, M.A

| Paper Code: CHEM-DSE-203B                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |             |           |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------|-----------|
| <b>Course Title:</b> Advance Organic Chemistry Theory<br><b>Contact Hrs:</b> 4 Lectures per Week<br><b>Examination Duration (Hrs.):</b> Two Hours<br><b>Mode of Evaluation:</b><br><b>Continuous Assessment (CA):</b> 10 Marks<br><b>End term Examination (ETE):</b> 40 Marks<br><b>Total Credits:</b> 4<br><b>Semester:</b> II<br><b>Subject Area:</b> Application of Organic Chemistry<br><b>Objective:</b> To acquire knowledge about industrial application of organic chemistry; organic molecule as a organic material, drug and polymer. |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |             |           |
| Unit                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            | Contents                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | Contact Hrs |           |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | L           | T         |
| 1                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | <b>Industrial Applications of Organic Chemistry:</b> Value-added chemicals from non-renewable resources and further organic transformations. Natural gas: conversion to value-added chemicals and materials. Chemicals derived from renewable resources: Source, value-added chemicals, and products. Bulk preparation methods. Industrial chemicals derived by the Fermentation process. Surface Active Agents, detergents, and pharmaceuticals.                                                                                                                                                                                                                                                                                                                                             | 15          | 5         |
| 2                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | <b>Organic Materials (Materials Chemistry):</b> Molecular electronics: molecular materials for electronics and molecular scale electronics: Molecular properties, molecular arrangement and molecular interactions, piezoelectric and pyroelectric organic materials; molecular magnets based on transition metal complexes and organic ferromagnets, organic non-linear optical materials: photochromic organic materials and their classes; conducting polymers: polyacetylene, polypyrrole, polyaniline and polythiophene; conductive charge transfer materials: TTTCNQ, metal-dithiolate systems, fullerenes. Langmuir-Blodgett films, molecular electronic logic and architectures.                                                                                                      | 15          | 5         |
| 3                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | <b>Synthesis and Uses of the following Drugs of different Pharmacological Activities:</b><br>j. Antimalerials: Quinine, Chloquine, Trimethoprim<br>k. Analgesic & Antipyretics: Paracetamol, Meperidine, methadone, Aminopyrine.<br>l. Anti-inflammatory: Aspirin, Ibuprofen, Oxyphenylbutazone, Diclophenac, Indomethacin, coxib, celecoxib.<br>m. Antitubercular and antileprotic: Ethambutol, Isoniazide & Dapsone<br>n. Anaesthetics: Lidocaine, Thiopental.<br>o. Antihistamines: Phenobarbital, Diphenylhydramine.<br>p. Tranquilizers: Diazepam, Trimeprazine<br>q. Cardiovascular: Synthesis of diltiazem, quinidine, methyl dopa, atenolol, oxyprenol<br>r. Anti-neoplastic drugs: Cancer chemotherapy, Synthesis of mechloaethamine, cyclophosphamide, Mephalan, uracils, mustards. | 15          | 5         |
| 4                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | <b>Organic and Inorganic Polymer:</b><br><b>Organic Polymer:</b> Manufacturing process, general properties, compounding and applications of SBR, Polyisoprene, Polybutadiene, Butyl rubber, Ethylene-propylene rubber, Neoprene rubber, Speciality rubbers: Silicon rubbers, Nitrile rubbers, Polyacrylic rubbers – Polyurethane rubbers – foam rubber.<br><b>Inorganic Polymers:</b> Classification of inorganic polymer, inorganic polymerisation reactions (addition, condensation and coordination polymerisation). Polysiloxanes, polysilanes, poly phosphazenes, polymeric sulfur. Synthesis, structure, properties and application of coordination polymers & organometallic polymers.                                                                                                 | 15          | 5         |
| <b>Total Contact Hours</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | <b>60</b>   | <b>20</b> |

**Recommended Books:**

1. M. A. Benvenuto, Industrial Organic Chemistry, Berlin, Boston: De Gruyter, 2017.
2. B. G. Reuben, J. S. Plotkin, H. A. Wittcoff, Industrial Organic Chemicals, Wiley, 3rd Edition, 201
3. H. H. Szmant, Organic Building Blocks of the Chemical Industry, Wiley & Sons, 1989.
4. E. R. Riegel, J. A. Kent. Riegel's Handbook of Industrial Chemistry, 2007
5. P.J. Vander Put, Inorganic Chemistry of Materials, Plenum Press, New York, 1998.
6. M.C. Petty, M.R. Bryce and D. Bloor, Editors An Introduction to Molecular Electronics, Edward Arnold, London 1995.
7. A. Kar, Medicinal Chemistry, New Age publications.

8. Thomas Nogrady, Donald F. Weave, Medicinal Chemistry-A Molecular and Biochemical Approach, Oxford University Press.
9. Burger. Medicinal Chemistry and Drug Discovery, Vol-1, Ed. M. E. Wolff, John Wiley (1994).
10. Goodman & Gilman. Pharmacological Basis of Therapeutics, McGraw-Hill (2005).
11. S. S. Pandeya & J. R. Dimmock. Introduction to Drug Design, New Age International. (2000)
12. D. Lednicer. Strategies for Organic Drug Synthesis and Design, John Wiley (1998).
13. Graham & Patrick. Introduction to Medicinal Chemistry (3rd edn.), OUP (2005).
14. C. Tanford, Physical Chemistry of Macromolecules, Wiley, Newyork, 1961
15. V.R. Gowariker, Polymer Science, New Age International New Delhi, 1986
16. Y. Morai, Micelles: Theoretical and Applied Aspects, Plenum (1992).
17. G. Odien, Principles of Polymerization, 3rd edition (1991) John Wiley & Sons, Singapore.
18. P. Bahadur and N.V. Sastry, Principles of Polymer Science, (2002) Narosa, New Delhi.
19. F.W. Billmayer, Jr., Text Book of Polymer Science, 3rd Edition (1984), Wiley-Interscience, New Y

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| <b>Paper Code: CHEM-DSE-203C</b>                                                                                                                                                                                             |
| <p><b>Course Title:</b> SWAYAM MOOCs Course.</p> <p>To be selected in the Departmental committee meeting by choosing one of the courses offered by the SWAYAM.</p> <p><b>Total Credits:</b> 4</p> <p><b>Semester:</b> II</p> |

**Paper Code: CHEM-DRP-204**

**Course Title:** Dissertation/Research Project/Entrepreneurship

**Contact Hrs:** 24 hours per Week

**Examination Duration (Hrs.):** Two Hours

**Mode of Evaluation:**

**Submission of Dissertation:** 100 Marks

**Presentation:** 30 Marks

**Viva-Voce:** 20 Marks

**Total Credits:** 12

**Semester:** II

**Subject Area:** Topic selection in consultation with the teacher, literature search from different reference books and using internet search, typed written-up with proper tables, structures, figures and literature to be submitted, seminar lecture on this topic to be delivered in presence of external expert and internal teachers.

**Objective:** To acquire knowledge about the advance research.