DEEN DAYAL UPADHYAYA GORAKHPUR UNIVERSITY

GORAKHPUR

Two Year M.Sc. Degree Course in

CHEMISTRY

(For session 2024 onwards)

Course Structure (Two Year PG Programme-2024) Total Credits- 92

The following are the papers in M.Sc. Chemistry course:

M.Sc. I Semester

(4 theories+1 Practical of 4 credits each)

Paper No.	Paper Name	Max. Marks	No. of Credits
CHE-501N (Core)	Molecular Symmetry and Molecular Vibrations	100	4+0
CHE-502N (Core)	Quantum Chemistry-I	100	4+0
CHE-503N (Core)	Main Group Elements	100	4+0
CHE-504N (Core)	Organic Reaction Mechanism	100	4+0
CHE-505N (Core)	Practical	100	0+4
		Total	**20**

M.Sc. II Semester

(4 theories+1 Practical and 1 open elective of 4 credits each)

Paper No.	Paper Name	Max. Marks	No. of Credits
CHE-507N (Core)	Analytical Chemistry	100	4+0
CHE-508N (Core)	Thermodynamics and Electrochemistry	100	4+0
CHE-509N (Core)	Transition Elements	100	4+0
CHE-510N (Core)	Natural Products	100	4+0
CHE-511N (Core)	Practical	100	0+4
Open Elective#		100	4+0
CHE-541N	Chemical Techniques	100	4+0
CHE-542N	Green Chemistry	100	4+0
		Total	**24**

any one of these paper for other PG Programmes

M.Sc. III Semester

(4 theories+1 Practical and 1 research project of 4 credits each)

Paper No.	Paper Name	Max. Marks	No. of Credits	Specialization
CHE-513N (Core)	Spectroscopy-I	100	4+0	**Theory-1** (Compulsory Paper)
CHE-514N	Quantum Chemistry-II	100	4+0	**Theory-2** (Any one of these papers)
CHE-515N	Chemical Applications of Symmetry and Group Theory	100	4+0	
CHE-516N	Stereochemistry	100	4+0	
CHE-517N	Electronics and Electrochemical Phenomena	100	4+0	**Theory-3** (Any one of these papers)
CHE-518N	Coordination Chemistry	100	4+0	
CHE-519N	Pericyclic and Rearrangement Reactions	100	4+0	
CHE-520N	Thermodynamics and Intermolecular forces	100	4+0	**Theory-4** (Any one of these papers
CHE-521N	Supramolecular Chemistry	100	4+0	
CHE-522N	Biomolecules	100	4+0	
CHE-523N	Practical	100	0+4	
CHE-524N	Research Project	100	0+4	
		Total	**24**	

M.Sc. IV Semester

(4 theories+1 Practical and 1 research project of 4 credits each)

Paper No.	Paper Name	Max. Marks	No. of Credits	Specialization
CHE-525N (Core)	Spectroscopy-II	100	4+0	**Theory-1** (Compulsory Paper)
CHE-526N	Chemical Kinetics, Solid State and Reaction Dynamics	100	4+0	**Theory-2** (Any one of these papers)
CHE-527N	Bioinorganic Chemistry	100	4+0	
CHE-528N	Organic Synthesis	100	4+0	
CHE-529N	Statistical Mechanics	100	4+0	**Theory-3** (Any one of these papers)
CHE-530N	Organo-Transition Metal Chemistry	100	4+0	
CHE-531N	Selected Topics in Organic Chemistry	100	4+0	
CHE-532N	Polymer Chemistry	100	4+0	**Theory-4** (Any one of these papers
CHE-533N	Inorganic Materials	100	4+0	
CHE-534N	Drugs and Agrochemicals	100	4+0	
CHE-535N	Solid State Chemistry	100	4+0	
CHE-536N	Nuclear and Radiation Chemistry	100	4+0	
CHE-537N	Biophysical Chemistry	100	4+0	
CHE-538N	Computational Chemistry	100	4+0	
CHE-539N	Practical	100	0+4	
CHE-540N	Research Project	100	0+4	
		Total	**24**	

Semester-I

CHE-501N: Molecular Symmetry and Molecular Vibrations

(4+0 Credits)

Course Objectives: Symmetry strictly defines relations between molecular spectra and molecular structure. This paper focuses on the mathematical tools which are necessary to apply symmetry concepts to vibrational spectroscopy.

Unit-1

Symmetry elements and symmetry operations with special reference to water and ethane. Classification of molecules/ ions based on their symmetry properties.

Unit-2

Derivation of matrices for rotation, reflection, rotation-reflection and inversion operations, Symmetry point groups applied to all type of molecules (C_{nh}, D_{nh}, C_{nv}, T_d, O_h and I_h).

Unit-3

Group multiplication basis, matrix representation, character of an operation, orthogonality, character tables, reducible and irreducible representations, groups, subgroups and classes.

Unit-4

Symmetry of normal vibrations, determination of normal modes by internal and Cartesian coordinates methods, mixing of internal coordinates in normal modes, selection rules for IR and Raman spectroscopy.

Unit-5

Normal coordinate analysis of water and ammonia molecules and their infrared and Raman spectral activity.

Books Recommended:

1. D.M. Bishop, "Group theory and Chemistry" Dover Publications.
2. F.A. Cotton, "Chemical Applications of Group Theory", John Wiley, 1971.
3. M. Hamaresh, "Group theory and its Applications to Physical Problems" Addison- Wisley
4. McWeeny, "Symmetry - An Introduction to Group Theory", Pergamon Press.
5. Lowell H. Hall "Group Theory and Symmetry in Chemistry", McGraw Hill Book Company, New York, 1969

6. K.VeeraReddy,"Symmetry and Spectroscopy of Molecules", New Age International Limited Publisher, New Delhi.

Course Outcomes:

CO 1: Symmetry elements and symmetry operations covers a wide area of research in theoretical chemistry.

CO 2: Understanding of symmetry of normal vibrations, determination of normal modes, mixing of internal coordinates and normal coordinate analysis of molecules develops the basis of experimental infra red and Raman spectroscopic analysis of molecules and their theoretical calculations via computational programmes.

CHE-502N: Quantum Chemistry I

(4+0 Credits)

Course Objectives: The objective of the course is to know the application of quantum mechanics in physical models and experiments of chemical systems. It is also called molecular quantum mechanics.

Unit-1

Fundamental Concepts:

- **a.** Operators and algebra of operators, commutators, Linear operators, Vector operators, Laplacian operators, Hermitian operators, Concept of normalization and orthogonality in wave function.
- **b.** Postulates of quantum mechanics.
- **c.** Schrodinger equation and particle in one dimensional and three-dimensional box and degeneracy of states.

Unit-2

Quantum mechanical treatment:

a. Quantum mechanical treatment of a harmonic oscillator, One dimensional Harmonic oscillator (Classical and quantum mechanical treatments), Energy levels of harmonic and an-harmonic oscillators.
b. Quantum mechanical treatment of a rigid rotor
c. Rigid rotor model of a diatomic molecule, Energy levels of a rigid rotor, Rigid rotor selection rule, A non rigid rotor.

Unit 3

Schrodinger equation for H atom:

Transformation of coordinates, Separation of Variables, φ,Θ and R equations and their solutions, Spherical harmonics.

Unit 4

Many –Electron Atoms:

Antisymmetry and Slater determinant for the wave function of ground state of multielectron atom, Self consistent field approximation (Hartree's Theory).

Unit 5

Approximation methods:

The variation method, Perturbation method and First order Perturbation theory.

Reference Books:

1. Quantum Chemistry by Donald A. Macquarrie
2. Molecular Quantum Mechanics by P.W. Atkins and R.S. Friedman
3. Quantum Chemistry by R. K. Prasad
4. Introductory Quantum Chemistry by A. K. Chandra
5. Quantum Chemistry by Ira N. Levine
6. Physical Chemistry by T. Engel and P. Reid

Course Outcomes:

CO 1: Students will be able to grasp fundamental concepts of operators, algebra of operators and quantum mechanical and Schrodinger wave equations for single and multi electron systems.

CO 2: Real analysis covers a wide area of research in computational chemistry. This course is useful in various completive exams like CSIR-NET, IAS, PCS.

CHE-503N: Main Group Elements

(4+0 Credits)

Course Objectives: The paper of main group elements is introduced to M.Sc. classes for the study of s and p block elements of the periodic table. The core objective of this paper is to prepare the students to understand and correlate preparation, structure, bonding and properties of s and p block elements.

Unit-1

Stereochemistry of Bonding in Main Group Components:

dπ – pπ bonds, Bents rule, Energetics of hybridization

Unit-2

Preparation, Structure, Bonding and Technical Applications of,

a. Polyether complexes of alkali and alkaline earth metals
b. Polyphasphazenes
c. Thiazyl and its polymers, tetrasulfur dinitride.

Unit-3

a. Structure and bonding of Borane anions
b. Classification and structures of Silicates

Unit-4

Synthesis and structure of:

a. Carbides
b. Polyions of Ge, Sn, Pb, Sb, Bi and Hg

Unit-5

a. Definition and classification of organometallic compounds on the basis of hapticity and polarity of metal-carbon bond
b. Preparation, Properties, Structure and Applications of **a**lkyl and aryls of Lithium, Beryllium, Aluminum, Mercury and Tin.

Reference Books:

1. Advance Inorganic Chemistry, 6th Edition, Cotton and Wilkinson
2. Inorganic Chemistry, 4th Edition, Principles of Structure and Reactivity by J.F. Huheey, E.A. Keiter and R.L. Keiter, 1993

3. Chemistry of Elements by N.N. Greenwood and A. Ernshaw, Butterworths 1997
4. Organometallic Chemistry: A Unified Approach by R.C. Mehrotra and A.K. Singh
5. Comprehensive Coordination Chemistry Vol.3 by G. Wilkinson, R.D. Gillard, And J.A. McCleverty, Pergamon Press 1987.

Course Outcomes:

CO 1. Students will be able to demonstrate an intuitive understanding of correlation between electronic configuration and bonding properties of elements.

CO 2. Chemistry of main group elements covers a wide area of research in inorganic chemistry.

CHE-504N: Organic Reaction Mechanism

(4+0 Credits)

Course Objectives:

1. Train students to grasp basics of organic reactions- step by step sequence of elementary reactions by which overall chemical change occurs.
2. To understand principles of organic reaction mechanism, substitution, elimination, homo- and hetero bond addition reactions.
3. To prepare the students for further research in organic chemistry.

Unit-1

Basic principle of organic reaction mechanism:

Potential energy diagram, methods of determination of organic reaction mechanism and their applications, kinetic isotopic effect and its importance in determination of reaction mechanism.

Unit-2

Substitution Reactions:

a. **Aromatic electrophilic substitution:** General view, energy profile diagram, arenium ion mechanism (ArSE) of different aromatic electrophilic substitution reactions, ipso-substitution and ortho/ para ratio.
b. **Aromatic nucleophilic substitution:** (ArSN) Addition- elimination and elimination- addition (benzyne) mechanisms,

c. **Aliphatic nucleophilic substitution:** Mechanism and stereochemistry of S_N1, S_N2, S_N' and S_N^i reactions, role of substrate's. Nuleophilic substitution at bridged head carbon atom.

d. **Neighouring group participation (NPG):** Evidence for NGP, participation of sigma., Pi- bonds, halogen, N-atoms and phenyl ring.

Unit-3

Elimination reaction:

E_1, E_2 and E_1cb mechanisms, orientation (Saytzef's and Hoffmann eliminations), pyrolytic (syn) elimination, stereochemistry of E_2 reaction, factors affecting E_1, E_2 and E_1cb reactions, Competition between substitution and elimination reactions.

Unit-4

C=C Bond Addition :

Mechanism and stereochemistry of addition of halogen and halogen acids to alkenes,1,2-hydroxylation, oxymercuration-demercuration, Corey epoxidation and cyclopropanation, Simmon-Smith cyclopropanation and Sharpless asymmetric epoxidation (SAE).

Unit-5

C-Hetero multiple Bond addition:

Mechanism of hydrolysis of ester and amide. Crame's rule. Condensation reaction involving Cannizzaro, Claisen and Knovenagel.

Reference Books:

1. Advanced Organic Chemistry Part. A & B By F. A. Carey and R. J. Sundberg, Plenum Publisher , New York, 2007.
2. Advanced Organic Chemistry By J. March, 2007.
3. Organic chemistry By J. Clayden, N. Greeves, S. Warren and P. Wothers, Oxford University Press , New York, 2001.

Course Outcomes: Organic reaction mechanism is the backbone of classical and applied organic chemistry.

Semester-I

CHE-505N: Practical

(0+4 Credits)

Marks (Practical) : 100; Time: 8 hrs in two days;

Marks distribution (Practical)

Practical: 75 marks

Internal Assessment: 25 marks

Physical Chemistry exercises:

1. Determination of the solubility of benzoic acid in water at different temperatures and calculate the heat of solution
2. Determination of the distribution coefficient of benzoic acid between benzene and water
3. Determination of the distribution coefficient of acetic acid between benzene and water
4. Determination of the distribution coefficient of iodine between carbon tetrachloride and water
5. Study the adsorption of acetic acid on charcoal and draw the Freundlich isotherm

Inorganic Chemistry exercises:

Qualitative analysis of an inorganic mixture of seven radicals including Tl, W, Se, Te, V, Be, U, Ti, Zr, Th, Ce and Li, in addition to the radicals prescribed for the B.Sc. course. Semi-micro analysis is to be done.

Organic Chemistry exercises:

Preparation of organic compounds involving two stages. Emphasis should be given in the following processes:

Purification, distillation under reduced pressure, steam distillation and fractional crystallization.

Semester-II

CHE-507N: Analytical Chemistry

(4+0 Credits)

Course Objectives:

1. To study concepts and theories behind basic methods and techniques used in analytical chemistry. This theory can be used to solve many rigorous problems of universe.
2. To prepare the students for further research in analytical methods of chemistry.

Unit-1

Electroanalytical Techniques:

a. **Conductometric:** Discussion of the nature of the curves of acid-base (including mixtures of acids), precipitation and complexometric titrations
b. **Potentiometric:** Different types of electrodes, discussion of the nature of the curves for oxidation-reduction and acid-base titrations, comparision with the conductometric method
c. **Voltametry:** Cyclic voltametry
d. **Polarography:** Dropping mercury electrode and its advantages, polarographically active species, concept of residual, diffusion and limiting current of half wave potential, Ilkovic equation and factors affecting diffusion current

Unit-2

Thermoanalytical Methods:

a. **Thermogravimetry:** Apparatus, factors affecting TG, Interpretation of TG curves of $CaC_2O_4.H_2O$ and $MgC_2O_4.2H_2O$
b. **Differential Thermal Analysis and Differential Scanning Calorimetry:** Apparatus, factors affecting DTA and DSC curves with special reference to heating rate, particle size and packing, measurement of heat of transition, heat of reaction and heat of dehydration of salts and metal hydrates.

Unit-3

Radiochemical Methods

a. Isotope method
b. Inverse isotopic dilution
c. Neutron activation technique

Unit-4

Chromatographic Method:

a. Gas Chromatography: GLC and GSC
b. HPLC

Unit-5

Spectral Methods:

a. Nephelometry
b. Turbidimetry
c. Flame Photometry

Reference Books:

1. Fundamentals of Analytical Chemistry: D.A. Skoog, D.M. West and F.J. Holler, 1992, 6e
2. Quantitative Inorganic Analysis, A.I. Vogel, 2012, 7e
3. Instrumental Methods of Chemical Analysis: B.K. Sharma, 2011
4. Instrumental Methods of Chemical Analysis: H. Kaur, 2016, 12 e
5. Analytical Chemistry, Gary D. Christian, 2007, 6e
6. Instrumental Methods of Analysis: H.H. Willard, L.L. Merrit, Jr. J.A. Dean, 1974, 5e

Course Outcomes:

After studying this course the student will be able to,

CO 1. Understand the basic of this course and think & develop new ideas and concepts in analytical chemistry

CO 2. Know about electroanayltical, thermoanalytical, radiochemical, chromatographic and spectral techniques.

CHE-508N: Thermodynamics and Electrochemistry

(4+0 Credits)

Course Objectives: The main objective of the course is to provide fundamentalconcepts of thermodynamics effects and relationships. The course is to give knowledge of comprehensive and rigorous treatment of classical thermodynamics, thermodynamics relations. Explain the concept of partial molar properties fugacity and activity. The course is designed to give an insight of phenomena of electrolytic conductance, reactions in solutions, basic principles of electrical phenomena are important for interfaces and electrode processes.

Unit 1

a. Some important thermodynamic effects and relationships :

The Joule Thomson's effect, The Gibbs Helmoltz equation and its application, The ClausiusClapeyron equation, The Maxwell's relation.

b. Partial molar Properties

Partial molar quantities, (partial molar volume and partial molar Gibbs energy), Chemical potential and variation of chemical potential with temperature and pressure, The Gibbs Duhem equation

c. Fugacity and Activity

Fugacity, variation of fugacity with temperature and pressure, Activity and the activity coefficient.

Unit 2

The Third law Thermodynamics:

The third law, Nernst heat theorem, application of third law, The residual entropy.

Unit 3

Electrolytic Conductance of strong electrolytes:

Debye-Falkenhagen effects, Wein effects the ionic association, effect of ionic strength on rate of ionic reactions.

Unit 4

Electrical phenomena at interface:

The electrical double layer, electrokinetic phenomena, quantitative treatment of electro osmosis, Electrophoresis and streaming potential.

Unit 5

Electrode processes:

Dissolution and deposition potential, decomposition potential and its determination, Concentration Polarization and over voltage (hydrogen overvoltage and oxygen overvoltage), The Limiting current density.

Reference Books:

1. Thermodynamics for Chemists by S. Glasstone.
2. An Introduction of Chemical Thermodynamics by R.P.Rastogi and R.R. Mishra.
3. Thermodynamics by K.S. Pitzer
4. Electrochemistry by S. Glasstone
5. Electrochemistry by Potter
6. Modern Electrochemistry by Bockris Reddy VoL I&II
7. Comprehensive Physical Chemistry by N.B. Singh, S.S. Das and N.S. Gajbhiye, New Age International Publishers.

Course Outcomes:

CO 1. To understand various thermodynamic relationship, the concept of free energy and partial molar quantities, activity and activity coefficients and determination.

CO 2. To understand the phenomena of electrolytic conductance. Reactions in solutions.

CO 3. To understand electrical phenomena at interfaces and electrode processes.

CO 4. To understand application of electrochemistry in electrolytic processes.

CHE-509N: Transition Elements

(4+0 Credits)

Course Objectives:

1. Train students to grasp fundamental chemistry of transition metal elements-group of element whose atom has a partially filled *d* sub-shell.
2. To understand principles of structure, stereochemistry, kinetics and mechanism of transition metal elements.
3. To prepare the students for further research in transition metal chemistry.

Unit-1

Structures of 2 to 8 Coordinate Metal Complexes:

Cation-anion ratio in various polyhedral, Hybrid orbitals and preferred conditions of formation of the complexes of following geometries :

C.N.2 - Linear

C.N.3 - Trigonal planar, Trigonal pyramidal

C.N.4 - Tetrahedral, Square planar

C.N.5 - Trigonal bipyramidal, Square pyramidal, pentagonal.

C.N.6 - Octahedral, Trigonal prism

C.N.7 - Pentagonal bipyramidal, Capped octahedral, Capped trigonal prism.

C.N.8 - Cubic, Tetragonal antiprismatic, Dodecahedral, Hexagonal bipyramidal, and Bicapped trigonal prism,

Stereochemical non-rigidity in four to eight coordinate Complexes.

Unit-2

Stereoisomerism in six coordinate octahedral complexes (Ma3bcd, Ma2bcde, Mabcdef and complexes containing bi-and ter- dentate ligands, Intermolecular and intramolecular rearrangements (Bailar and Ray Dutta twist only), mechanism of racemisation in tris (chelate) octahedral complexes, Methods of resolution of optical isomers.

Unit-3

Kinetics and mechanism of substitution reactions in octahedral Co (III) and square planar Pt (II) complexes.

Unit-4

Mechanism of one electron transfer reactions (inner and outer sphere mechanisms), Factors affecting the rates of direct electron transfer reactions and the Marcus equation, Two electron transfer reactions.

Unit-5

Metal Ligand Equilibria in Solution:

Step wise and overall formation constants and their relations, Factors affecting the stability of metal complexes with reference to the nature of metal ions and ligands, determination of stability constants by pH-metric and spectroscopic methods.

Books Recommended:

1. Inorganic Chemistry, 4th Edition, Principles of Structure and Relativity by J.E. Huheey, E.A. Keiter and R.L. Keiter, 1993
2. Chemistry of Elements by N.N. Greenwood and A. Ernshaw, Butterworths, 1997
3. Mechanism of Inorganic Reactions; A Study Of Metal Complexes in Solution by F. Bosolo and R.G. Pearson
4. Ligand Field Theory And Its Application by B.N. Figgis and M.A. Hitchman, Wiley, New York, 2000.

Course Outcomes: After studying this course the student will be able to,

CO 1. Understand the basic of transition metal chemistry and think & develop new ideas in this field.

CO 2. Know geometries of 2 to 8 coordinate metal complexes, streoisomerism, kinetics and mechanism of substitution reactions in octahedral and square planar complexes.

CO 3. Understand mechanism of electron transfer reactions and stability of transition metal complexes.

CO 4. Develop new ideas for further research in the field of coordination chemistry.

CHE-510N: Natural Products

(4+0 Credits)

Course Objectives: Natural product chemistry is branch of chemistry that deals with chemicalcompounds or substances produced by a living organism-that is, found in nature. Natural products can also be prepared by chemicalsynthesis (both semi synthesis and total synthesis) and have played a central role in the development of the field of organic chemistry by providing challenging synthetic targets.

Basic concepts and knowledge of chemistry of natural products are necessary to develop understanding of core organic chemistry i.e. simple to complex organic structures, organic structural determination, semi-synthetic to total synthetic pathways of organic structures etc.

Unit- 1

Acetogenins : Classification, general method of structure determination of,

- **a.** Flavones- Chrysin
- **b.** Flavonols – quercetin
- **c.** Anthocyanins- Cyanin
- **d.** Anthocyanidins- cyanidin chlorides

Unit-2

Terpenoids : Introduction, isolation and general methods of determining structure of,

- **a. Monoterpenoids**
- **i.** Acyclic monoterpenoids: Citral and geraniol
- **ii.** Monocyclic monoterpenoids : α-Terpineol

Unit-3

Alkaloids: Introduction and general methods of determining structure of,

- **i.** Hemlock alkaloid- Coniine
- **ii.** Pyrrolidine-Pyridine alkaloid- Nicotine
- **iii.** Chincona alkaloids -Quinine
- **iv.** Opium alkaloids : Papaverine and Morphine
- **v.** Rauwolfia alkaloids

Unit-4

Carbohydrates: Structure and functions of,

Disaccarides- Lactose, Sucrose

Unit- 5

Biosynthesis of natural products:

i. The acetate hypothesis, Isoprene rule, mevalonic acid from acetylco-enzyme – A, biogenesis of terpenoids
ii. Shikimic acid pathway of biogenesis of aromatic ring
iii. General biogenesis of alkaloids

Reference Books:

1. Organic Chemistry, I.L. Finar Vol. I and II, 2000
2. Natural Products, S.M. Chawla, 2018
3. Biochemistry-Lehninger, 2000
4. Biochemistry by L. Stryer, 1995

Course Outcomes: After studying this course the student will be able to,

CO 1. Understand basics of different classes of natural products- Acetogenins, Terpenoids, Alkaloids and Carbohydrates and their general structural determination.

CO 2. Know about acetate hypothesis, isoprene rule, biogenesis of – Terpenoid, aromatic ring (Shikimic acid pathway) and alkaloid.

CO 3. Develop ideas for further research total organic synthesis.

CHE-511N: Practical

(0+4 Credits)

Marks (Practical) : 100; Time: 8 hrs in two days;

Marks distribution (Practical)

Practical: 75 marks

Internal Assessment: 25 marks

Physical Chemistry exercises:

1. Solubility curve for water-acetic acid-chloroform systems
2. Determination of the rate constant of the acid-catalysed hydrolysis of ethyl acetate at laboratory temperature
3. Determination of the rate constant of the hydrolysis of ethyl acetate by sodium hydroxide at laboratory temperature
4. Conductometric titration between strong acid and strong alkali
5. Determination of the dimerization constant of benzoic acid in benzene medium by partition method

Inorganic:

Either both gravimetric and one volumetric, one gravimetric estimation of two metal ions from following mixtures:

a. Cu^{+2} and Ni^{+2}
b. Cu^{+2} and Zn^{+2}
c. Ni^{+2} and Zn^{+2}
d. Cu^{+2} and Ba^{+2}
e. Cu^{+2} and Ag^{+}
f. Fe^{+2} and Ag^{+}
g. Ba^{+2} and Ag^{+}

Organic:

Analysis of primary binary organic mixture (Liquid-Liquid, Liquid-Solid, Solid-Solid)

Semester-III

CHE-513N: Spectroscopy-I

(4+0 Credits)

Course Objectives: The paper of spectroscopy-I is introduced to M.Sc. classes for the detailed studies of fundamental concepts, tools and techniques used behind UV-visible, infra red, Raman and diffraction methods for structural determination of molecules.

Unit-1

UV-Visible Spectroscopy :

Different type of electronic transitions, Lambert-Beer's law, Chromophores, Auxochromes, Solvent effect, Red shift and blue shift, Woodward's rule for conjugated cyclic and acyclic dienes and α, β – unsaturated carbonyl compounds, Absorption in aromatic compounds (substituted benzene, naphthalene and anthracene), Problems related to UV-Visible Spectroscopy.

Unit-2

Infrared Spectroscopy:

Linear harmonic oscillator, Vibrational energies of diatomic molecules, Zero point energy, Force constant and bond strength, Anharmonicity, Morse potential energy diagram, Selection rules, Overtones, Hot bands, Absorption by common functional groups, Brief description of IR and FTI.R instruments, Problems related to IR Spectroscopy.

Unit-3

Raman Spectroscopy:

Theories of Raman Effect, Conditions of Raman active vibrations, Selection rules, Polarized and depolarized Raman lines, Study of: (a) Simple molecules such as SO_2, CO_2, N_2O and C_2H_2; (b) Hydrogen bonding and (c) Metal ions in solution, Mutual exclusion principle, Problems related to Raman Spectra and its interpretation.

Unit-4

Diffraction Methods for Structure Determination

a. X-ray Diffraction: Principle, elucidation of crystal structure of NaCl by X-ray diffraction, Structure factor, Methods for structure determination by trial and error methods, Fourier's method of analysis and Patterson's function method.
b. Electron diffraction: Principle, technique, scattering intensity versus scattering angle curves, Wierl equation, energy electron diffraction (LEED)
c. Neutron diffraction: Principle, technique and difference with electron diffraction

Unit-5:

Common problems related to above spectroscopic techniques

Reference Books

1. Fundamentals of Molecular Spectroscopy, 4th Ed. Mc Graw-Hill, C.N. Banwell
2. Basic Principles of spectroscopy, Mc Graw –Hill, R. Chang
3. Organic Spectroscopy, ELBS, W. Kemp
4. Modern Spectroscopy, Wiley, J.M. Hollas

Course Outcomes: After studying this course the student will be able to,

CO 1. Understand the basics of UV-visible, infra red, Raman and diffraction methods techniques.

CO 2. Solve numerical and experimental graphs of all of the above techniques.

CO 3. Cover wide area of research in above spectroscopic methods.

CHE-514N: Quantum Chemistry- II

(4+0 Credits)

Course Objectives:

1. To understand atomic and molecular structure and properties, as well as chemical reactivity.

2. To develop a knowledge and understanding of the concept that quantum states live in a vector space.

3. To relate this abstract formulation to wave and matrix mechanics.

4. To develop a knowledge and understanding of perturbation theory, level splitting and radiative transitions.

5. To develop a knowledge and understanding of the role of angular momentum in atomic and nuclear physics.

6. To develop a knowledge and understanding of the relation between conservation laws and symmetries.

7. To solve quantum mechanical problems.

Unit-1

Symmetry Properties and Quantum Mechanics

Invariability of schrodinger Equationfor a molecule with respect to symmetry operations and its consequences. Construction of molecular orbitals of ammonia and pie molecular orbitals of naphthalene, The direct product representation and its application in the derivation of selection rules for electronic, vibrational and Raman spectra.

Unit-2

Huckel Molecular Orbital Theory Of con jugated systems and its Applications

Calculation of energy levels and delocalisation energy of butadiene, cyclic conjugated systems: cyclopropenyl, cyclobutadiene, cyclopentadienyl, benzene, concept of aromaticity and antiaromaticity, Huckel treatment of linear polyenes.

Unit-3

Semi- Empirical and Ab-Intio SCF Theories

Semi- empirical SCF theory (CDNO, INDO & MNDO), Slater and Gaussian type orbitals, Configurational interaction and electron correlation , Moeller- Plasset Perturbation methods.

Unit-4

Introduction to Density Functional Theory :

Concept of basis sets, The Hohenberg variational theorem and Kohn- Sham orbitals, The Local Density Approximation (LDA) and Generalized Gradient Approximation (GGA). Density Functional theory and it significance.

Unit-5

Molecular Mechanics

A brief introduction to molecular mechanics.

Reference Books:

1. Introductory Quantum Chemistry by A. K. Chandra
2. Quantum Chemistry by R. K. Prasad
3. Molecular Quantum Mechanics by Atkins and Friedman
4. Quantum Chemistry by Ira N. Levine, Prentice Hall of India, New Delhi 1995
5. Chemical Application of Group Theory by F. A. Cotton

Course Outcomes:

CO 1. Increasing the accuracy of the results for small molecular systems, and increasing the size of large molecules that can be processed, which is limited by scaling considerations.

CO 2. Foundation of quantum mechanics to remind the difference between classical and quantum world.

CO 3. See how operator algebra can be used to solve simple eigenvalue problems.

CO 4. Understanding what is meant by the orbital concepts.

CO 5. The role of rotational and spin angular momentum in chemistry.

CO 6. Be able to use approximate methods in solving molecular problems.

CO 7. To master molecular orbital theory in diatomic and polyatomic molecules.

CHE-515N: Chemical Application of Symmetry and Group Theory

(4+0 Credits)

Course Objectives: The objective of the paper is to provide a systematic study of symmetry in any chemical system by using mathematical framework.

Unit-1

Symmetry and Point Groups

Definitions, the symmetry point groups, identification of molar point groups, molecules of low symmetry, high symmetry and special symmetry (C_n , S_n, D_n, C_{nv}, and D_{nh} only)

Unit-2

Groups, Sub-Groups, Classes and Matrices Representation

Definitions, multiplication tables, group generating elements, sub-groups and classes, irreducible representations, the orhtogonality Theorem.

Matrix Representations of symmetry elements, block-factorization of larger matrices, matrix representation of C_{3v}, and C_{4v}, point groups, transformation matrices.

Unit-3

Normal Modes of Vibrations

Cartesian Coordinate and internal coordinate methods of normal mode analysis applied to C_{2v} (Symmetric XY_2, ZXY_2), C_{3v} (XY_3), T_d (XY_4) and O_h (XY_6) systems.

Unit-4

Valence Bond treatment and Molecular Orbitals

Formation of hybrid orbitals of XY_3 (planar), XY_4 (tetrahedral and square planar), Molecular Orbitals ofA_2 and AB_n (n= 1 to 3) type molecules.

Unit-5

Crystal Fields

Derivation of 'd' orbital splitting patterns of central atom (M) in ML_2, ML_3, ML_5, and ML_7 system (energy calculations are not required). The effect of weak crystal field on S, P, D, F and G spectroscopic terms in Oh and Td point groups.

Books Recommended:

1. F. A. Cotton, "Chemical aAplications of Group Theory". 2nd Ed..Wiley Eastern. 1971.
2. L. H. Hall, "Group Theory and Symmetry in Chemistry", McGraw Hill Inc.. 1969.
3. M. Orchin and H. H. Jaffe, "Symmetry, Orbitals and Spectra, Wiley Interscience. 1971.
4. C.J. Ballhausen and H. B. Gray, "Molecular Orbital Theory", W. A. Benzamin Inc. 1965.
5. K.Veera Reddy," Symmetry and Spectroscopy of Molecules", New Age International Limited Publisher, New Delhi.

Course Outcomes: Once the symmetry of a molecule is analyzed, significant features of many chemical and physical properties of that molecules can easily be determined by using the tool of Group Theory. These applications are useful to predict aboutthechirality, chemical bonding and molecular orbital of a given molecule. It's vibrational motions and spectroscopic transitions etc. can also be studied.

CHE-516N: Stereochemistry

(4+0 Credits)

Course Objectives: Stereochemistry is sub discipline of chemistry, involves the study of the relative special arrangement of atoms that form the structure of molecules and their manipulation. It spans the entire spectrum of organic, inorganic, physical, biological and supramolecular chemistry and hence understanding of stereochemistry is needed to develop idea of complex chemical structures and asymmetric organic synthesis.

Unit-1

Stereoisomerism with chiral centre:

Chirality, molecules with more than one chiral centers, interconversion of Fischer, Newman and saw-horse projections and absolute configuration.

Unit-2

Stereoisomerism with axial/ planar chirality and Helicity:

Principle of axial and planar chirality; optical isomerism of biphenyl,allenes and spiranes; optical activity due to intramolecular crowding and their absolute configuration.

Unit-3

a. Topo city and pro-stereo isomerism:

Introduction; homotropic, enantiotropic and diastereotropic atoms, groups and faces; Nomenclature and symbols.

b. **Cyclostereoisomerism**

Configuration and conformations; stability of mono- and disubstituted cycloheaxanes and cyclohexanones, Chirality of disubstituted cyclohexane.

Unit-4

Assymetric Synthesis:

- **a.** Regioselective , stereoselective and sterospecefic reactions.
- **b.** Asymmetric synthesis involving chiral auxillary , chiral reagent and chiral catalysis.
- **c.** Enantioimeric excess.

Unit-5

Stereochemistry of compounds containing **S** and **P** atoms and geometrical isomerism of compound containing -C=N and -N=N- bonds.

Reference Books:

1. Stereochemistry of carbon compounds by E. L. Eliel, 1997
2. Stereochemistry by P. S. Kalsi, 1997
3. Stereochemistry of Organic compounds By D. Nasipuri, 1994

Course Outcomes: After studying this course the student will be able to,

CO 1. Have understanding of various classes of stereoisomers -axial and planar chirality, helicity, topocity and pro-streoisomerism and cyclostreoisomerism.

CO 2. Fundamental terms and concept behind advance organic synthesis- asymmetric synthesis.

CO 3. Develop ideas for further research in asymmetric synthesis.

CHE-517N: Electrodics and Electrochemical Phenomena

(4+0 Credits)

Course Objectives: The main objective of the course is to provide impart advanced knowledge of electrodics and electrochemical phenomena. The course is designed to get insight of electrical double layer, corrosion, polarization resistance and conductance in non-aqueous media.

Unit1

Conductance in non-aqueous media

Ion dissociation, its effect on conductance, diffusion of electrolytes, measurements of diffusion coefficient, in relation to conductance

Unit-2

Electrical Double Layer Theory

The Helmholtz –Perin Theory, The Gouy- Chapman Theory, Stern Modification in the Gouy-Chapman Theory.

Unit-3

Electrodics

The equilibrium exchange current density, Butler Volmer Equation, Tafel plot, high field and low field approximation, Electrodeposition and electropolymerization.

Unit-4

Corrosion

The mechanism of corrosion of metals, corrosion current and corrosion potential, Electro- chemical corrosion theory, corrosion prevention.

Unit-5

Polarization Resistance

Polarisation, Classification of polarisation phenomena, polarisation curves, Polarisation resistance and linear polarisation.

Reference Books:

1. Electrochemistry by S. Glasstone
2. Electrolytic Solutions by Robinson& Stokes
3. Electrochemistry by Potter
4. Modern Electrochemistry by Bockris and Redd : Vol I and II
5. Electro Chemical Impedance Spectroscopy by Mc Donald
6. Theoretical Electrochemistry by L.I. Antropov

Course Outcomes: The students will acquire knowledge of :

CO 1. Conductance in non-aqueous media

CO 2. Various models of electrical double layer

CO 3. Butler- Volmer equation, Tafel plot, electro-deposition and electro-polymerization.

CO 4. Prevention and mechanism of corrosion of metals, chemical corrosion theory, corrosion current and corrosion potential, polarization resistance.

CHE-518N: Coordination Chemistry

(4+0 Credits)

Course Objectives: The main objectives are,

1. To understand energy level in an atom, free ions in crystal field, electronic spectra, magnetic properties and metal ligand bonding in transition metal complexes.
2. To prepare the students for further research in coordination chemistry.

Unit-1

Energy levels in an atom:

Relation between electronic configuration and energy terms, Hund's rules and ground state energy terms. Inter electron repulsion parameter. Variation of Racah B and C parameters in different transition series. Spin orbit coupling parameters.

Unit-2

Free ions in crystal fields:

Effect of weak crystal field on free ion terms in octahedral, square planar and tetrahedral symmetries. Orgel diagrams, Mixing of terms, Medium and strong field approximation in Oh point group, transition from weak to strong field and correlation diagram for only d^2 case, Non-crossing rule, Tanabe Sugano diagrams.

Unit-3

Electronic spectra of complexes:

Interpretation of the spectra of aqueous solution of $[M(H_2O)_6]^{n+}$, calculation of Dq, B and β parameters, Jahn Teller distortion and its effect on electronic spectra.

Unit-4

Magnetic properties of Complexes:

Dia, para, ferro and antiferromagnetism, Quenching of orbital angular momentum by ligand . The magnetic properties of A, E and T terms.

Unit-5

Metal-ligand Bonding:

Limitations of CFT, Nephelauxetic series, molecular orbital energy level diagram of octahedral, tetrahedral and square planer complexes.

Books recommended:

1. B.N. Figgis, M.A. Hitchman, Ligand Field Theory and Its Applications, Willey, New York, 2000
2. D. Sutton, Electronics Spectra of Transition Metal Complexes, Mc-Graw-Hill, London, 1968.
3. K. Veera Reddy, Symmetry and Spectroscopy of Molecules, New Age Inter Pvt. Ltd., New Delhi, 1999.

Course Outcomes:

CO 1. Students will be able to demonstrate an intuitive understanding ofconcepts of coordination chemistry.

CO 2. Coordination chemistry covers a wide area of research in inorganic chemistry and hence this course willmotivate students to enhance their knowledge in this field via research.

CHE-519N: Pericyclic and Rearrangement Reactions

(4+0 Credits)

Course Objectives: The paper of pericyclic and rearrangement reactions is introduced to M.Sc. classes for the detailed studies of rearrangement reactions and concerted (pericyclic) reactions.

Unit-I

Carbocation rearrangements:

Wagner- Meerwein, Tiffeneau- Demjanov & Dienone- phenol rearrangements.

Unit-2

Carbanion rearrangements:

Sommelet- Hauser , Stevens , Favorskii and Wittig rearrangements.

Unit-3

Rearrangements to electron deficient N- and O-atoms

Hoffmann , Curtius , Lossen , Schmidt, Beckmann rearrangements & Baeyer-Villiger oxidation

Unit-4

Pericyclic Reactions (Electrocyclic & Cycloaddition):

Characteristics and classification of pericyclic reactions. Conservation of M. O's symmetry, correlation, FMO and PMO methods forthe study of following reactions:

a. **Electrocyclic reaction**: Study of linear conjugated dienes and trienes systems
b. **Cyclo-addition reaction:** [2+2] and [4+2] systems, detailed study of Diel's-Alder reaction

Unit-5

Pericyclic Reactions (Sigmatropic & chelotropic reactions):

a. **Sigmatropic shift:** Study of [1,3]; [1,5] and [3,3] and higher order sigmatropic shifts Claisen –rearrangement; Cope, oxy-Cope and aza-Cope's rearrangements
b. **helotropic and Group transfer reactions**. General introduction and mechanism.

Reference Books:

1. Advanced Organic Chemistry Part. A & B By F. A. Carey and R. J. Sundberg, Plenum Publisher ,New York, 2007
2. Organic chemistry By J. Clayden, N. Greeves, S. Warren and P. Wothers, Oxford University Press , New York, 2007
3. Advaced Organic Chemistry By J. March, 2007
4. Pericyclic Reactions By Mukharjee and Singh, 2001

Course Outcomes:

CO 1. Students will be able to have applied understanding of various pathways of organic rearrangement reactions and pericylic reactions.

CO 2. Thiscourse is useful in various competitive exams like CSIR-NET, GATE, IAS, PCS etc.

CHE-520N: Thermodynamics and Intermolecular Forces

(4+0 Credits)

Course Objective: The objective of this paper is:

1. To introduce students to Intermolecular Forces including the process like dispersion, dipole, induction and Charge transfer forces, hydrogen bond.
2. To introduce students to how to solve Excess thermodynamic functions, Regular solutions, Solution of macromolecules, Activity Coefficient determination by NRTL and UNQUAC Models, ASOG and UNIFAC methods.

3. To introduce students to how to explore thermodynamic relations at lamda - point. Thermodynamic interpretation of phase diagrams: Eutectic systems, Systems exhibiting complete miscibility in solid and liquid phases, Mixtures having a congruent melting point, Critical solution mixing
4. To study about Configurational entropy and free energy, Cell theory of liquid state, Entropy production in irreversible processes, Entropy equation for heat flow, relation between fluxes and forces, non- equilibrium stationary states, Linear phenomenological equations, Onsager's reciprocity relation, non –linear thermodynamic treatment of electro- kinetic phenomena, thermo- osmosis and reverse osmosis.

Unit-1

Intermolecular Forces

Dispersion, dipole, induction and Charge transfer forces, The hydrogen bond.

Unit-2

Thermodynamics of Mixture

Excess thermodynamic functions, Regular solutions, Solution of macromolecules, Activity Coefficient determination by NRTL (Non Random Two Liquids) and UNQUAC (Universal Quasi chemical Approach) Models, ASOG (Analytical Solvents of Groups) and UNIFAC (Universal functional Activity Coefficient) methods.

Unit-3

Phase Equilibria

Thermodynamic relations at lamda - point. Thermodynamic interpretation of phase diagrams: Eutectic systems, Systems exhibiting complete miscibility in solid and liquid phases, Mixtures having a congruent melting point, Critical solution mixing.

Unit-4

Liquid State

Configurational entropy and free energy, Cell theory of liquid state, Hole theory, Molecular theory of liquid viscosity, mesomorphism.

Unit-5

Thermodynamics of Irreversible Processes

Entropy production in irreversible processes, Entropy equation for heat flow, relation between fluxes and forces, non- equilibrium stationary states, Linear phenomenological equations, Onsager's reciprocity relation, non –linear thermodynamic treatment of electro- kinetic phenomena, thermo- osmosis and reverse osmosis.

Reference Books:

1. Introduction to thermodynamics of irreversible processes by I. Prigogine.
2. Non –Equilibrium Thermodynamics in Biophysics by A. Katchalsky and P.F. Curran.
3. Thermodynamics of Irreversible processes by S.R. DeGroot.
4. Thermodynamics by E.A. Guggenheim.
5. Introduction to Non Equilibrium physical chemistry by R.P. Rastogi.
6. Thermodynamics-A core course by R.C. Srivastava, Subit K. Saha and A.K. Jain.
7. The Thermodynamics of Steady States by K.G. Denbigh.
8. Thermodynamics by Pitzer.
9. Regular solutions by J.H. Hilderbrand and R.L. Scott.

Course Outcomes:

On completion of the course the students,

CO 1. know the forces which applies in between the molecules and hydrogen bond

CO 2. will be able to make intelligent choices of thermodynamic mixtures.

CO 3. knows phase equilibrium.

CO 4. has knowledge of Configurational entropy and free energy, Molecular theory of liquid viscosity,

CO 5. is able to explore the irreversible process by the means of thermodynamics.

CHE-521N: Supramolecular Chemistry

(4+0 Credits)

Course Objectives: Supramolecular chemistry is the discipline covering "the chemistry of molecular assemblies and of the intermolecular bond" and deals with "organized entities that result from the association of two or more chemical species held together by intermolecular forces. This paper is introduced to M.Sc. classes for the detailed studies of general principles of molecular recognition, complex formation and host design, templates and self assembly through various examples and applications.

Unit-1

Definition, classification of supramolecular host-guest compounds, nature of

supramolecular interactions, Chelate and macrocyclic effects, General principles of molecular recognition, complex formation and host design, templates and self assembly.

Unit-2

Host-Guest Chemistry (Cation Binding Hosts):

i. Crown ethers
ii. Cryptands
iii. Spherands

Unit-3

Host-Guest Chemistry (Anion Binding Hosts):

i. Expanded porphyrins
ii. Guanidinium Based reseptors

Unit-4

Host-Guest Chemistry (Neutral Molecules Binding Hosts):

i. Solid State Clatharates
ii. Zeolites

Unit-5

Selected Applications in:

a. Catalysis
b. Ion Transport
c. Molecular switches, rectifiers and Molecular wires

Books Recommended

1. Supramolecular Chemistry: concepts and perspectives by J. M. Lehn, 1995
2. Supramolecular Chemistry by JW Steel and JL Atwood, 2004
3. Principles and Methods in Supramolecular Chemistry by H Scheneider and A Yatsimirsky, 2000
4. Supramolecular Chemistry: an Introduction by F Vogtle, 1993
5. Perspectives in Supramolecular Chemistry, Vol.2, Crystal Engineering and molecular recognition by Desiraju (Ed.), 2003

Course Outcomes: After studying this course student will be able to,

CO 1. Have understanding of theories behind supramolecular interaction and various classes of host-guest chemistry and its applications.

CO 2. Develop ideas for further research in the field of supramolecular chemistry.

CHE-522N: Biomolecules

(4+0 Credits)

Course Objectives: The main objectives are,

1. Train students to understand interdisciplinary areas of chemistry in a lucid and effective manner.
2. To understand vitamins, steroidal harmones and steroids.
3. To prepare the students for further research in areas covering Chemistry and Biology.

Unit-1

Water Soluble Vitamins:

Structure and Physiological functions of the followings water soluble vitamins-

a. **Non B- Complex Vitamin** -Vitamin C
b. **B -Complex Vitamins**- Thiamine B_1, Riboflavin B_2

Unit- 2

Fat Soluble Vitamins:

Structure and Physiological functions of the followings fat soluble vitamins.

a. Vitamin A : Retinol
b. Vitamin E : Tocoferol
c. Vitamin K : Vitamin K_1

Unit- 3

Steroidal Hormones:

a. General introduction to estrogens and androgens
b. Oestrone (Estrone) : Structure and synthesis, relationship to Oestradiol (estradiol)
c. Progesterone: Preparation from steroid and physiological functions

Unit- 4

Non Steroidal Hormones

Structure and Physiological functions of Thyroxin and Adrenalin

Unit- 5

Steroids:

Diels hydrocarbon, Determination of ring system, positions of hydroxyl group, angular methyl group, double bond, nature and position of side chain in cholesterol., synthesis of cholesterol

Reference Books:

1. Biochemistry by Lehninger, 2007
2. Organic Chemistry by I. L. Finar Vol. II, 2004
3. Biochemistry by Lubert Stryer, 2008

Course Outcomes: After studying this course student will be able to,

CO 1. Understand the basic of this course and think & develop new ideas in this course.

CO 2. Know structure and physiological function of water soluble and fat soluble vitamins, steroidal and non-streiodalharmones, and steroids.

CO 3. Cover a wide area of research in chemical-biology and/or biological-chemistry.

CHE-523N: Practical (Physical)

(0+4 Credits)

Marks (Practical) : 100; Time: 8 hrs in two days;

Marks distribution (Practical)

Practical: 75 marks

Internal Assessment: 25 marks

Excercises:

1. pH-metry:

a. Determination of strength of strong acid and strong base
b. Determination of strength of weak acid by pH-titration with a strong base
c. Verification of Henderson's equation

2. Conductometry

a. Equivalent conductance of strong electrolytes at infinite dilution
b. Conductometric titration of weak acid with strong base
c. Titration of mixtures of acids
d. Precipitation titration
e. Verification of Ostwald's dilution law
f. Verification of Kohlrausch's law

3. Potentiometry

CHE-524N : Research Projects* (Physical)

(0+4 Credits)

Project Titles:

1. CMC of surfactants by surface tension measurement.
2. Determination of molecular weight of polymer by Rast method.

*Under the research project, the student can conduct experiments, engage in review writing, perform lab work, or complete dissertation work related to the syllabus of a particular semester, all under the supervision of the assigned mentor.

CHE-523N: Practical (Inorganic)

(0+4 Credits)

Marks (Practical) : 100; Time: 8 h in two days;

Marks distribution (Practical):

Practical: 75 marks, Internal Assessment: 25 marks

Exercises:

1. **EDTA Titration**:
   Estimation of Mg^{+2}, Zn^{+2}, and Mg^{+2}, Ca^{+2} in a mixture.

CHE-524N: Research Projects* (Inorganic)

(0+4 Credits)

Project Titles:

1. Separation and gravimetric estimation of ternary metal systems.
2. Estimation of metal ions in polluted water.

*Under the research project, the student can conduct experiments, engage in review writing, perform lab work, or complete dissertation work related to the syllabus of a particular semester, all under the supervision of the assigned mentor.

CHE-523N: Practical (Organic)

(0+4 Credits)

Marks (Practical) : 100; Time: 8 h in two days;

Marks distribution (Practical):

Practical: 75 marks, Internal Assessment: 25 marks

Exercises:

1. Multistep synthesis of organic compounds
2. Estimation of glycine

CHE-524N: Research Projects* (Organic)

(0+4 Credits)

Project Titles:

1. Estimation of elements in organic compounds.

*Under the research project, the student can conduct experiments, engage in review writing, perform lab work, or complete dissertation work related to the syllabus of a particular semester, all under the supervision of the assigned mentor.

Semester-IV

CHE-525N: Spectroscopy-II

(4+0 Credits)

Course Objectives: The paper of spectroscopy-II is introduced to M.Sc. classes for the detailed studies of fundamental concepts, tools and techniques used behind mass-spectrometry, nuclear magnetic resonance, electron spin resonance and Mossbauer spectroscopy methods for structural determination of molecules.

Unit-1

Mass Spectrometry

Measurement technique (El, Cl, FD and FAB), Molecular base and molecular ions, various class of organic molecules, McLafferty re-arrangement and retro-Diels-Alder Fragmentation, nitrogen rule and determination of molecular composition of organic compounds from mass spectra data.

Unit-2

^{1}H-NMR

The spinning nuclei, Chemical shift and its measurement, factors affecting chemical shifts, anisotropic effect and shielding mechanism, interpretation of protons spin-spin coupling, coupling constant, simple, virtual and complex coupling, Chemical and magnetic equivalence, NMR studies of other nuclei e.g., ^{19}F and ^{31}P, application in structural determination of simple organic and inorganic molecules.

Unit-3

^{13}C-NMR

General introduction, peak assignments, chemical shift, ^{13}C-^{1}H coupling, Off-resonance Decoupling, Deuterium, fluorine and phosphorus coupling, NOE and DEPT, 2D NMR, Application to simple organic and inorganic molecules.

Unit-4

Electron Spin Resonance Spectroscopy

Basic principle, factor affecting value, isotropic and anisotropic hyperfine coupling constant, Application to organic free radical, Methyl free radical, Naphthalene and Benzene free radicals, CID NP.

Unit-5

Mossobauer Spectroscopy

Theory, Instrumentation, Applications - isomer shift, nuclear quadrupole coupling and hyperfine interaction, Problems related toMossobauer Spectroscopy.

Reference Books:

1. Fundamentals of Molecular Spectroscopy, 4th Ed. Mc Graw-Hill, C.N. Banwell
2. Basic Principles of spectroscopy, Mc Graw –Hill, R. Chang
3. Organic Spectroscopy, ELBS, W. Kemp
4. Modern Spectroscopy, Wiley, J.M. Hollas

Course Outcomes: After studying this course the student will be able to,

CO 1. Understand the basics of mass-spectrometry, nuclear magnetic resonance, electron spin resonance and Mossbauer spectroscopy.

CO 2. Solve numerical problems and experimental graphs of all of the above techniques.

CO 3. Cover wide area of research in above spectroscopic methods.

CHE-526N: Chemical Kinetics, Solid state and Reaction Dynamics

(4+0 Credits)

Course Objectives:

1. To provide a simple and general description of Unit 1-3.

2. To provide an introduction of Limitation of Lindemann theory, Hinshelwood treatment, RRK theory (salient features and limitations) RRKM theory and advances made by Slater.

3. To give knowledge of collision cross-section, Inter- molecular potential, potential energy surfaces and elastic molecular collisions.

Unit-1

Chemical Kinetics

The study of fast reaction: Flow system, Relaxation and shock tube methods, Flash photolysis

Unit-2

Oscillatory Chemical Reactions

Autocatalysis, Autocatalytic Mechanisms of oscillatory chemical reaction : The lotka Volterra mechanism, The Brusselator, the Oregonator, Bistability and Chemical chaos.

Unit-3

Solid State

Thermodynamics of Schottky and Frankel Defects, Synthesis, Characterization and Applications of Nanomaterials; Solid State Reaction.

Unit-4

Statistical Treatment of Unimolecular reaction

Limitation of Lindemann theory, Hinshelwood treatment, RRK theory (salient features and limitations) RRKM theory and advances made by Slater.

Unit-5

Reaction Dynamics

Collision cross-section, Inter- molecular potential, potential energy surfaces and elastic molecular collisions.

Reference Books:

1. Solid State Chemistry by D.K. Chakrabarty. New Age International (P) Limited, Publishers, New Delhi.
2. Molecular Reaction Dynamics by R.D. Levine, R.B. Bernstein.
3. Dynamics by N. Sathyamurthy
4. Theories of Chemical Reaction rate by K.J.Laidler.
5. Physical Chemistry, Walter J. Moore

Course Outcome:

CO 1. Students will get ability to of fast reaction: Flow system, Relaxation and shock tube methods, Flash photolysis

CO 2. The students will be able to understand Autocatalytic Mechanisms of oscillatory chemical reaction: The lotka Volterra mechanism, The Brusselator, the Oregonator, Bistability and Chemical chaos.

CO 3. Students will be aware of Thermodynamics of Schottky and Frankel Defects, Synthesis, Characterization and Applications of Nanomaterials; Solid State Reaction.

CO 4. Students will be able to understand the Limitation of Lindemann theory, Hinshelwood treatment, RRK theory (salient features and limitations) RRKM theory and advances made by Slater.

CO 5. Students will acquire an ability to learn Collision cross-section, Inter- molecular potential, potential energy surfaces and elastic molecular collisions.

CHE-527N: Bioinorganic Chemistry

(4+0 Credits)

Course Objectives: Bioinorganic chemistry is a field that examines the role of metals in biology. Bioinorganic chemistry includes the study of both natural phenomena such as the behavior of metalloproteins as well as artificially introduced metals, including those that are non essential, in medicine and toxicology. This paper is introduced to M.Sc. classes for the detailed studies of interdisciplinary area of biology and inorganic chemistry.

Unit-1

Metalloenzymes:

Zinc enzymes - carboxypeptidase, carbonic anhydrase; Copper enzymes - superoxide dismutase; Mobybdenum - xanthine oxidase; Coenzyme vitamin B_{12} , Biological nitrogen fixation, molybdenum nitrogenase, other nitrogenase model systems.

Unit-2

Bioenergetics and ATP cycle:

Glucose storage, metal complexes in transmission of energy, chlorophylls, Photosystem I and II in cleavage of water.

Unit-3

Transport and Storage of Dioxygen:

Heme proteins and oxygen uptake, Structure and function of hemoglobin, myoglobin, hemocyanins and hemerythrin, model synthetic complexes of iron.

Unit-4

Electron Transfer, Metal Storage and Transport:

Structure and function of metalloproteins in electron transport process - cytochromes and iron - sulphur proteins, synthetic models, Ferritin, transferrin and siderophores..

Unit-5

Metals in Medicine:

Metal deficiency and diseases, toxic effects of metals, metals in chemotherapy with particular reference to anticancer drugs.

Books Recommended:

1. Bioinorganic Chemistry. R. N. Hay. Wiley. 1984.
2. The Inorganic Chemistry of Biological Processes. M. M. Hughes. Wiley 1981.
3. An Introduction to bioinorganic Chemistry. El Ichiro Ochai. Allyn. 1977.
4. Inorganic Chemistry : Principles of structure and reactivity. J.E. Huheey Harper. 1983.
5. Advanced inorganic Chemistry. F.A. Cotton and G. Wilkinson. Wiley. 1999.

Course Outcomes: After studying this course the student will be able to,

CO 1. Have ideas of metalloenzymes, bioenergetics, transport and storage of dioxygen, electron transfer, metal storage and metals in medicine.

CO 2. Cover wide area of research in above topics.

CHE-528N: Organic Synthesis

(4+0 Credits)

Course Objectives:

1. Train students to grasp advances in organic synthesis- applications of selective name reactions and catalysts used in synthetic organic laboratories.
2. To prepare the students for further research in organic chemistry.

Unit-1

Selective named reactions and their applications in organic synthesis:

Barton, Bayllis–Hillman, Hoffmann-Lofferer-Fretag, Michael addition, Mitsonubu, Nazaro Mannich,Julia & Peterson olefination ,Robinson annulations, Reformatsky, Shapiro, Stork-enamine

Unit-2

Oxidation:

Scopes of the following reagents with applications and mechanisms: SeO_2, Jones reagent , PCC , PDC, Swern oxidation and iodobenzene diacetate.

Unit-3

Reduction:

Scope,Mechanism and stereochemistry of reduction with following reagents-

$NaBH_4$, LAH, DIBALH and Birch reduction.

Unit-4

Reagents:

Preparation and uses of following reagents in organic synthesis.

a. Gillman, DCC, DDQ , LDA, Diazomethane, Bu_3SnH and 1,3-dithiane (unpolung)

b. Sulphur and phosphorous Ylids.

Unit-5

Pd(0) and Pd(II) complex in organic synthesis: Heck , Suzuki,Stille and Sonogashira reactions,

Reference Books:

1. Organic Synthesis By Michael B Smith , Mc-Graw Hill, 2001
2. Advanced Organic Chemistry Part. A & B By F. A. Carey and R. J. Sundberg, Plenum Publisher , New York, 2002
3. Advanced Organic Chemistry By J. March, 2007
4. Organic chemistry By J. Clayden, N. Greeves, S. Warren and P Wothers, Oxford University Press, New York, 2007

Course Outcomes: Organic synthesis– reactions and catalysts is the backbone oforganic chemistry and will train students to develop ideas for further research in the field of synthetic organic chemistry..

CHE-529N: Statistical Mechanics

(4+0 Credits)

Course Objective:

1. To study the Basic of Classical Statistical Mechanics terminologies.
2. To study the Energy levels, Boltzmann distribution law, Fermi-Dirac statistics Bose – Einstein Statistics.
3. To study The partition functions, relation of the partition function of the thermodynamic function.
4. To study the unit 4 .
5. To study the Equilibrium Constants from partition function for: Isomerisationequilibrium,Ionisation- equilibrium (H↔H++e), and Dissociation equilibrium(Na2↔2Na).

Unit-1

Basic of Classical Statistical Mechanics

Phase space, Ensembles-average, Liouvilles theorem, Basic postulates, Classical limit, Quantisation of phase space.

Unit-2

Distribution laws

Energy levels, Boltzmann distribution law, Fermi-Dirac statistics Bose –Einstein Statistics.

Unit-3

Distribution & Thermodynamics

The partition functions, relation of the partition function of the thermodynamic function.

Unit-4

Determination of Partition functions

Localised and non-localised systems, Separation of the partition function. Translation partition function. The Sackur Tetrode-equation, Rotational partition function, vibrational partitionfunctions, Electronic partition function. Derivation of thermodynamic properties of ideal gases from partition functions.

Unit-5

Applications

Equilibrium Constants from partition function for: Isomerisation equilibrium,Ionisation-equilibrium ($H \leftrightarrow H^+ + e$), and Dissociation equilibrium($Na_2 \leftrightarrow 2Na$)

Reference Books

1. Statistical Mechanics: N. Davidson
2. Statistical Mechanics: D.A. Mcquarrie
3. Thermodynamics: J.P. Holman
4. Theoretical Chemistry: S. Glasstone
5. Physical Chemistry: Fried, Blukis and Hameika

Course Outcomes:

At the end of the course, students will be able to

CO 1. have an understanding ofPhase space, Ensembles-average, Liouvilles theorem, Basic postulates, Classical limit, Quantisation of phase space.

CO 2. have an enhanced knowledge of Distribution laws, Distribution Thermodynamics.

CO 3. have sound knowledge of Determination of Partition functionsviz; Localised and non-localised systems, Separation of the partition function and other partition function.

CO 4. develop skills in application related to partition function like equilibrium, Ionisation-equilibrium and Dissociation equilibrium.

CHE-530N: Organo-transition Metal Chemistry

(4+0 Credits)

Course Objectives: Organo-transition metal chemistry is the study of chemical compounds containing at least one chemical bond between a carbon atom of an organic molecule and a transition metal. This paper is introduced to M.Sc. classes for the detailed studies of transition metal organometallic compounds, organotransition metal catalysts and basic ideas of fluxional organometallic compounds.

Unit-1

Alkyls and Aryls of Transition Metals:

Types, General Synthetic Routes, Stability and Decomposition pathways.

Unit-2

Compounds of Transition Metal - Carbon Multiple Bond: Carbenes and Carbynes:

Low valent carbenes and carbynes ,synthesis, nature of bond and Structural Characteristics.

Unit-3

Transition Metal π- Complexes:

a. Preparations, Important reactions relating on the ligands, Structural features and bonding of alkenes, alkynes, allyls, diene, dienyl, arene complexes, MO approach of bonding in ferrocene and bis (benzene) chromium.
b. Ligand behaviour of $C_3Ph_3^+$, $C_7H_7^+$ and $C_8H_8^{2-}$ in different organometallic compounds.
c. Substitution reactions in metal carbonylsd using σ-donor, σ-donor and **π** -acceptor and **π** -donor ligands.

Unit-4

Catalysis involving organometallic compounds:

Olefin hydrogenation. Oxo reaction. Fischer Tropsch process. Wacker process. Polymerisation of olefins.

Unit-5

Fluxional Organometallic Compounds:

Fluxionality and dynamic equilibria in compounds such as η^3 – allyl and η^1 dienyl complex.

Books Recommended:

1. Comprehensive Organometallic Chemistry, Ed. E.W. Abel, Abel, F.G.A. Stone and G. Wilkinson, Pergamon, 1982.
2. Advnaced Inorganic Chemistry, F.A. Cotton and G. Wilkinson, `Wiley, 1999.
3. The chemistry of elements, N.N. Greenwood and A. Earnshaw, 1997.
4. Inorganic Chemistry, principles of structure and reactivity. J.E. Huheey, Harper, 1983.
5. Organometallic Chemistry (A unified approach), R.C. Mehrotra and A. Singh, Wiley Eastern, 1991

Course Outcomes: After studying this course student will be able to,

CO 1. Acquire understanding of various classes of organotransition metal compounds-alkyl and aryls of transition metals, transition metal complexes of carbenes and carbynes and transition metal pi-complexes.

CO 2.Have understanding of catalysis reactions involving organotransition metal compounds and basics of fluxional organometallic compounds.

CO 3. Develop ideas for further research in the field of organotransition metal chemistry.

CHE-531N: Selected Topics in Organic Chemistry

(4+0 Credits)

Course Objectives: The paper of selected topics in organic chemistry is introduced to M.Sc. classes to have knowledge of aromaticity, protection and deprotection of groups, heterocycles and organic photochemistry.

Unit-1

Aromaticity:

Concept of aromaticity, anti-aromaticity, non-aromaticity and homoaromaticity. Alternant and non- alternant systems. Aromaticity in non-benenoids (tropolone, azulene , annulenes, ferrocene and fullerene)

Unit-2

Protection and Deprotection of Groups:

Principle of protection and deprotection of alcohols, thiols and 1,3-diols, amines, carbonyls and carboxyl groups in organic synthesis.

Unit-3

Heterocycles:

General introduction and nomenclature.Chemistry of:

a. **Five membered:** Pyrazole& imidazole; and thiazole&iso-thiazole
b. **Six membered:** Pyrazine, pyrimidine and pyridaze

Unit-4

Organic Photochemistry:

Electronically exited states, spin-multiplicity, Jablonski diagram

a. **Photochemistry of Alkenes:** Geometrical isomerization, cyclic diamerization and photo-oxidation reaction. Reactions of 1,4 and 1,5- dienes (di-pi methane and related rearrangements)
b. **Photochemistry of Aromatic compounds:** Skeletal isomerization, isomerization of disubstituted benzenes. photo-Fries rearrangement.

Unit-5

Photochemistry of Carbonyl compounds:

Reduction, inter and intramolecular addition (Patterno-Buchi) Fragmentation (Norish-1 and Norish-11).Reaction of saturated acyclic, cyclic and unsaturated carbonyl compounds.

Reference Books:

1. Advanced Organic Chemistry Part. A & B By F. A. Carey and R. J. Sundberg, Plenum Publisher, New York, 2007
2. Advanced Organic Chemistry By J. March, 2007
3. Organic chemistry By Clayden, Greeves, Warren and Wothers, Oxford University Press , New York, 2007
4. Molecular Reactions and photochemistry By C. H. Depay and O.L. Chapman, 2001

Course Outcomes: After studying this course student will be able to,

CO 1. Have understanding of ideas of aromaticity and protection and deprotection of groups which is essential component of synthetic organic chemistry.

CO 2. Have knowledge of organic photochemistry, an advance branch of organic chemistry.

CHE- 532N: Polymer Chemistry

(4+0 Credits)

Course Objectives: Polymer chemistry is a sub-discipline of chemistry that focuses on the chemical synthesis, structure, chemical and physical properties of polymers and macromolecules. The principles and methods used within polymer chemistry are also applicable through a wide range of other chemistry sub-disciplines like organic chemistry, analytical chemistry, and physical chemistry and hence introduced in M.Sc. IV semester classes.

Unit-1

Basic Concepts and Polymer Characterization

General definition, Types and Classification of polymers, Concept of average molecular weights in polymers: (Number average, Weight average, Viscosity average and Sedimentation average molecular weights), Concepts of Mono-dispersity, poly-dispersity, Significance of Molecular Weight, Distribution Curves of polymers.

Unit -2

Polymerization

Kinetics and mechanism of condensation, Addition (Radical chain and Ionic chain), Coordination and Copolymerization.

Unit-3

Degradation of Polymers

Types of degradation: Random degradation and Chain depolymerisation, A general idea of thermal, mechanical and oxidative degradation, Antioxidants and stabilizers.

Unit-4

Rheology of Polymers

Viscous flow (Newtonian and Non- Newtonian fluids),Rubber elasticity (thermodynamic and entropy, elasticity), Visco-elasticity, The glassy state and glass transition temperature.

Unit-5

Polymer Processing

Plastic Technology: A general idea of Moulding and Extrusion techniques, Thermoforming and Thermofoaming.

Fiber Technology: A brief idea of textile and fabric terms and properties of fibers, Fiber Spinning techniques (melt, wet and dry spinnings).

Reference Books:

1. F.W. Billmeyer,"Textbook of Polymer Science", John Wiley &Sons, New York.
2. H.R.Allcock, F.W.Lampe and J.E Mark, "Contemporary Polymer Chemistry", PearsonEducation Prentice Hall, Singapore.
3. Charles E. Cariaher, "Polymer Chemistry:An Introduction", Marcel Dekker Inc, New York.
4. U.R.Gowariker, N.V.Vishwanathan and J. Shreedhar,"Polymer Science", New Age International Publishers, New Delhi.
5. S.S.Das and N.B.Singh,An Introduction to Polymer Science and Technology", New age International Publishers, New Delhi.

Course Outcomes: After studying this course student will be able to,

CO 1. Have detailed ideas of polymer chemistry- characterization, polymerization, degradation, rheology and processing.

CO 2. Develop ideas for further research in the field of polymer chemistry.

CHE-533N: Inorganic Materials

(4+0 Credits)

Course Objectives:

Inorganic materials are in the very focus of current worldwide research interest as highly promising material candidates for various forefront applications. Spectacular phenomena such as luminescence, photoconductivity, laser applications, semi conductions, super conduction have already been uncovered for these materials. The objective of this course is to study synthesis, properties and applications of these materials.

Unit-1

Lattice Defects:

Introduction to types of solids, Perfect and imperfect crystals, point defects, line defect and plane defect (definition and explanation of meaning), Schottky and Frenkel defect,

Nonstoichiometric defect (structural aspects), incorporation of stoichiometric excess defects, Magnetism due to defects (soft and hard magnetic materials).

Unit-2

Synthesis of Inorganic Materials:

Synthesis of solid state materials using different techniques (ceramic techniques, co-precipiattion techniques, sol-gel techniques, precursor techniques).

Unit-3

Properties of Materials

a. Optical Properties

Introduction, Optical properties of metals and non-metals, Luminescence, Photoconductivity, Lasers, non linear optical materials and optical fibers in communications.

b. Electrical Properties

Electrical conduction, Conduction in term of free electron and band theory. Semiconductors -Intrinsic and Extrinsic semiconductors and semiconductor devices.

Introduction of superconductors, High Tc super conductivity in Cuparates, preparation and characterization of 1-2-3 and 2-1-4 materials, Theory of superconductivity. Application of high Tc materials.

Unit-4

Nano Materials:

Introduction, preparation of nano materials, size property relationship, Carbon nanotubes, application of nano materials.

Unit-5

Metal clusters:

Conditions for formation of metal-metal bond. Carbonyl type clusters. Electron count in metal clustures, Isopoly and heteropoly acids and salts of Cr, V, Mo.

Books Recommended

1. A.F. Wells, Structural Inorg. Chem., ELBS & Oxford Univ. Press, 1975
2. C.N.R. Rao, A Muller & A.K. Cheetham, The Chemistry of nano-Materials, Wiley-VCH, Vol. 1 and Vol. 2, 2004.

3. F.A. Cotton, G. Wilkinson, C.A. Murillo, M. Bochmann, Advanced Inorg. Chem., John-Wiley & Sons, 1999.
4. J.E. Huheey, G.A. Keiter, R.L. Keiter, Inorg. Chem.: Principles of Structures and Reactivity, Harper Collins College Publishers, 1993.
5. D.M. Bruce, Inorganic Materials, 5 Volume sets, Wiley, 2011.
6. U. Schbert, N. Husing, Synth. of Inorg. Materials, Wiley, 2005.
7. D. Bahadur, Inorg. Materials: Recent Advances, Alpha Science International Ltd., 2004.

Course Outcome: After the course the students will be able to,

CO 1. understand lattice defects and synthesis of these materials

CO 2. understand applicable properties of Inorganic materials

CO 3. think and develop new ideas of these materials for optical, electrical and nanomaterial applications and further research into these fields.

CHE-534N: Drugs and Agrochemicals

(4+0 Credits)

Course Objectives: Topic of drugs and agrochemicals is included in M.Sc. classes due to its wide applicationin our daily life. Chemistry of drugs is an important discipline at the intersection of chemistry, especially synthetic organic chemistry, and pharmacology and various other biological specialties, where they are involved with design, chemical synthesis and development for market of pharmaceutical agents, or bio-active molecules (drugs).An agrochemical or agrichemical, a contraction of agricultural chemical, is a chemical product used in agriculture. In most cases, agrichemical refers to pesticides including insecticides, herbicides, fungicides and nematicides.

Unit- 1

Synthetic Drugs A:

A general methods of synthesis and applications of :

i. Sulpha drugs: Sulphanilamide, sulphathiazole, sulphathalidine, sulphasuccidine, sulphaguanidine, sulphapyridine
ii. Antimalarials: **(a)** 4-Aminoquinoline derivatives: chloroquine, santoquine **(b) 8-** aminoquinoline derivatives: Pamaquine, Pentaquine.

Unit- 2

Synthetic Drugs B:

A general introduction and applications of:

i. Anti-cancer agents: Nitrogen mustards, antimetabolites in cancer chemotherapy.
ii. Psychopharmacological agents: Synthesis and applications of promazine, chloropromazine, mepazine.
iii. Antitubercular agents: Synthesis and applications of Para Aminosalicylic Acid (PAS), Thiosemicarbazones, and hydrazides.

Unit- 3

Antibiotics:

Synthesis of penicillin-G, penicillin-V, chloramphenicol,

Unit- 4

Insecticides

i. A brief reference to natural insecticides, tobacco alkaloid, pyrothrins and rotenoids (detailed chemistry not required)
ii. Organophosphorus insecticides, OMPA, Parathion, malathion,
iii. Halogenated insecticides **,** halogenated alkanes, gammexane, DDT and important analogs (DFDT, DMDT, DDD).

Unit- 5

a. Fungicides:

Synthesis and applications of following agrochemicals

Halogenated phenols and quinones, dithiocarbamates, Zineb, Maneb, Ferbam

b. Herbicides

Synthesis and applications of 2,4-D and related compounds, substituted ureas and carbamates

Reference Books:

Medicinal Chemistry by A. Burger, 2002

Course Outcomes: After studying this course student will be able to,

CO 1. Have understanding of general method of preparation and applications of various classes of drugs- sulpha drugs, antimalarials, anti cancer agents, psychopharmacological agents, antitubercular agents and antibiotics.

CO 2. Develop ideas of agrochemicals- insecticides, pesticides, fungicides and herbicides.

Understanding chemistry of drugs and agrochemicals is the backbone of pharmaceutical and agrichemical industries and will train students to develop ideas for further research into these fields and advancement of their career towards chemicals industries.

CHE-535N: Solid State Chemistry

(4+0 Credits)

Course Objectives: The student will obtain required knowledge for understanding material science problems. Initially, they will study the structure of solids and get introduced with the importance of chemical and physical bonds, crystal (dis)order and defects for materials properties. They will get insight into electronic structure of crystals and compare it with the electronic structure of nanomaterials – to understand the 'nano' prefix. The student will understand high temperature phase equilibria and learn thermodynamic and kinetic treatments of phase transitions. They will learn synthesis design and planning, different processing technoques and their chemical-physical fundamentals as well as basic method of characterisation of solids.

Unit-1

Crystal Structures:

Rock salt, Zinc blende, Wurtzite, Daimond, Graphite, Fluorite, Sesquoide, Spinel (Normal/inverse), ReO_3, Perovskite, Amorphous state, quasi-crystals, Icosahedron, Silicates, Zeolites

Unit-2

Imperfections in crystals:

Point defects: Schottky and Frenkel defects, Colour centres line defects: Edge and screw dislocations, Burger's vector, dislocation densities, dislocation multiplicity and slip dislocation and crystal growth.

Surface imperfection: Grain boundaries

Unit-3

a. Semiconductors:

Intrinsic and impurity semiconductors, Carrier concentrations, Effect of temperature aon electrical conductivity and mobility of electrons in semiconductors, Hall effect, Seebeck coefficient, p-n junctions, Organic semiconductors

b. Superconductivity

Zero resistance and transition temperature, superconductivity and periodic table, Magnetic properties, Theory of superconductivity (BCS theory), Type I and Type II superconductors, Hard superconductors, Preparation of superconducting materials and their applications.

Unit-4

Phase transformations in solids:

Classification and thermodynamics of phase transformations in solids, Experimental methods of the study of phase transformations, Phase transformations in metals, Nucleation and crystal growth mechanism, Alloys, Some compounds such as titanium dioxide, aluminium oxide, dicalcium and tricalcium silicate, Dendritic growth, Preparation of single crystals from vapour, melt and solution.

Unit-5

Solid State Reactions:

Classification, Nature of solid state reactions, Reactions involving single solid phase, solid-gas reaction, solid-solid reaction, solid-liquid reaction, Intercalation chemistry, Reactions of organic solids, factors affecting solid state reactivity, Experimental methods for the study of solid state reactions

Reference Books:

1. Solid state chemistry and applications by A.R. West (2014. 2E)
2. Phase transitions in solids by K.J. Rao and C.N.R. Rao (1978)
3. Solid state chemistry by N.B. Hannay (1967)
4. Solid state chemistry by D.K. Chakrabarty (2010)

Course Outcomes: To obtain the knowledge on design and development of materials with pre-required properties based on understanding the structure of solids in its influence on physical-chemical properties, understanding of phase relations, chemical synthesis, reaction kinetics as well as characterisation methods.

CHE-536N: Nuclear and Radiation Chemistry

(4+0 Credits)

Course Objectives: The aim of this course is to give a thorough introduction to radioactivity as well as central concepts in radiochemistry. Radiochemical principles are seen in conjunction with chemical concepts and other fields where radiochemical principles can be utilized. Those examples are from e.g. industry, the environment and medicine. The course shall relay knowledge about the role of radioactivity, both as a tool and its own scientific discipline. Applications where radiochemistry plays an integral part will be specifically treated.

The course will contain the physical basis of nuclear structure and how the properties of the nucleus changes during radioactive decay. The different nuclear radiations, their interactions, and how they can be detected. Radiation properties and how these are used in chemical applications, and how different radiation interacts with matter. Many applications in the field of medicine,, especially positron emission tomography (PET) and nuclear medicine therapy will be discussed.

Unit-1

The Atomic Nucleus:

The atom, Units used in Nuclear chemistry, The nucleus and the outer sphere, classification of nuclides, nuclear stability, atomic energy.

Unit-2

Nuclear Models:

The shell model, The liquid drop model, The Fermi gas model, The collective model, The optical model.

Unit-3

Nuclear Reactions:

Bethe's notation, types of nuclear reactions, conservation in nuclear reactions, reaction cross section, the compound nucleus theory, experimental evidence of Bohr's theory, Experiments of Ghoshal, Alexander and Simonoff, Specific nuclear reactions, Photonuclear reactions, Direct nuclear reactions, Thermonuclear reactions.

Unit-4

Nuclear fission:

The process of nuclear fission, Fission fragments and their mass distribution, Charge distribution, Ionic charge of fission fragments, Fission energy, Fission cross-sections and thresholds, Fission neutrons, Theory of nuclear fission, The nuclear Reactors.

Unit-5

Radioactivity:

Radioactive elements, General characteristics of radioactive decay, Alpha decay, Beta decay, Nuclear deexcitation, gamma emission, artificial readioactivity

The Szilard-Chalmer's reaction, Radiochemical principles in the use of tracers, Uses of nuclear radiations, Radioisotopes as a source of electricity

Reference Books

Essentials of Nuclear Chemistry by Hari Jeevan Arnikar (1995)

Course Outcomes: The student,

CO 1. Can define radioactive decay processes and nuclear radiation

CO 2. Knows the principles of utilizing radioactivity applied to chemistry, chemical processes and adjacent fields where chemistry is an integral part.

CO 3. Knows the principles of radiation hygiene and the interaction of radiation and matter.

CO 4. Can update himself/herself on current methods in radiochemistry.

CHE-537N: Biophysical Chemistry

(4+0 Credits)

Course Objectives:

The objective of this course is to study biological systems using theories and concepts of physics and physical chemistry. The most common feature of this course is to seek explanation of the various phenomena in biological systems in terms of either the molecules that make up the system or the supra-molecular structure of these systems.

Unit-1

Biological Membranes:

Mechanism of facilitated diffusion of glucose, chloride ion and bicarbonate ion through erythrocytes, Mechanism of active transport of Na^+, K^+, Ca^{+2} and proton through membrane, co-transport: symport and antiport, Brief description of Na^+ channel protein and transport antibiotics. Brief description of molecular assembly and LB films

Unit-2

a. **Nucleic acids:**

Conformation of DNA and RNA (A,B and Z forms), Genetic code and gene-protein relationship, DNA cloaning and principle of protein engineering, DNA damage and repair mechanism

b. **Proteins:**

Conformation of polypeptide chain, periodic structures in proteins: α-helix, β-pleated sheet, collagen helix and β-turn, principle of protein folding and forces involved in protein folding Structures and functions of myoglobin, haemoglobin, lysozyme and carboxypeptidase A.

Unit-3

Bioenergetics:

The mechanism of oxidative phosphorylation-chemical coupling hypothesis, the conformational coupling hypothesis and chemi-osmotic coupling hypothesis

Unit-4

Biological Regulations:

Prostaglandins, cyclic AMP and its role in hormone action, Interferon

Unit-5

Enzyme Kinetics and Theory of Enzyme Catalysis:

Presteady state kinetics, steady state kinetics, kinetics of enzyme inhibitors and determination K_1, kinetics of multisubstrate enzyme-compulsory order, random order and double displacement type mechanism, non-linear enzyme kinetics

Reference Books:

1. Biophysics by M.V. Vallenstein, MIR publication, Moscow
2. Biochemistry by L. Stryer, Freeman and Co,, San Fransisco (Indian Print CBS Publications, Delhi).

3. Biophysical Chemistry Part I, II and III by C.R. Cantor and P.R. Schimmel, Freeman and Co., San Fransisco.
4. Principles of Biochemistry by Lehninger, Neloson and COX, Worth Publishers INC, US (Indian Print CBS Publishers, Delhi)
5. Enzyme Kinteics by P.C. Engel, Chapman and Hall, London

Course Outcome: After the course the students will be able to

CO 1. understand the basics of this course

CO 2. understand the use of this course in different field of science

CO 3. think and develop new ideas of biological systems- biological membranes, nucleic acids, proteins and grasp concepts and theories of physical chemistry-energetics, kinetics and catalysis to solve fundamental problems of biological systems.

CO 4. get benefit of this course while working in various national and international research laboratories of chemical-biology.

CHE-538N: Computational Chemistry

(4+0 Credits)

Course Objectives:

1. To discuss the basic principles of quantum mechanics, which are necessary to understand the properties of atoms and molecules and their chemical reaction.
2. A variety of different methods for the calculation of molecular properties will be systematically discussed.
3. To generate information that is complementary toexperimental data on the structures, properties, and reactions of substances for solving chemical problems.
4. To computing experimentally observed quantities, computational chemistry is also helpful in computing unobserved chemical phenomena.
5. A detailed physical and mathematical affirmation of a trend that hithertofound its boldest expression in the structural formulae of organic chemistry.

Unit-1

Introduction to Computational Chemistry and computable quantities (structure, potential energy surface, chemical properties)

Unit-2

Construction of z-matrix

- **a.** Diatomic molecules
- **b.** Polyatomic molecules
- **c.** Ring systems

Unit-3

Force Field/Molecular Mechanics

Potential energy functional forms

i. Common force fields viz., Harmonic, LJ (6-12), LJ(10-12) and More

ii. Existing force fields in popular packages viz., AMBER, CHARMM, DREIDING and MMn

Unit-4

Ab-initio HF calculations:

- **a.** Geometry optimization and calculation of HF energy
- **b.** Basis sets
- **c.** Density functional theory

i. Basic theory

ii. Advantage over *Ab-initio* approach

iii. Gaussian, Gamess & MOLPRO

iv. Applications

Unit-5

Applications to Real systems

- **a.** Biomolecules

i. Methods for modelling Biomolecules

ii. Site-specific interaction

iii. Introduction to computer aided Drug design (CADD)

- **b.** Synthetic route prediction
- **c.** Polymers/ smart materials
- **d.** Transition metals and clusters

Reference Books:

1. Introduction to computational chemistry by Frank, Jensen
2. Computational Chemistry by C.J. Cramer

Course Outcomes:

CO 1. Identify and explain the main similarities and difference between theoretical approach such as HF (Hartree-Fock), DFT (Density Functional Theory) and Molecular Mechanics (Force field methods).

CO 2. Describe and identify the various methods advantage/disadvantages for simulating/modelling various scientific problems.

CO 3. Choose and justify suitable methods for calculating electronic properties of simple molecules and crystals and be critically analysing the calculated properties.

CO 4. The program allows graphical input of molecular structure, menu-driven input to quantum chemistry calculational programs, and graphical analysis of molecular properties.

CO 5. Useful in analyzing theproperties of short-lived transition states and intermediates and species that are difficult to handle inside a laboratory such as explosives.

CO 6. Computational methods can be used to compute the properties of unknown moleculesand will be helpful in testing the properties of molecules in-silico before actualexperiment has been carried out.

CHE-539N: Practical (Physical)

(0+4 Credits)

Marks (Practical) : 100; Time: 8 h in two days;

Marks distribution (Practical)

Practical: 75 marks

Internal Assessment: 25 marks

Excercises:

1. **Chemical Kinetics**
    a. Determination of rate constant of acid hydrolysis of esters
    b. Relative strength of strong acids by studying the kinetics of hydrolysis of esters
    c. Kinetics of reactions between potassium persulphate and potassium iodide
    d. Kinetics of iodination of acetone
2. **Optical Methods**
    a. Spectroscopic methods of analysis: UV-visible, IR
    b. Polarimetry
    c. Refractometry

CHE-540N: Research Projects* (Physical)

(0+4 Credits)

Project Titles:

1. Spectrometry
2. Verification of Lambert Beer's Law by Colorimetry.
3. Determination of molar refraction by refractometer.
4. Electrodeposition of metals - $CuSO_4$, $ZnSO_4$

*Under the research project, the student can conduct experiments, engage in review writing, perform lab work, or complete dissertation work related to the syllabus of a particular semester, all under the supervision of the assigned mentor.

CHE-539N: Practical (Inorganic)

(0+4 Credits)

Marks (Practical) : 100; Time: 8 h in two days;

Marks distribution (Practical)

Practical: 75 marks

Internal Assessment: 25 marks

Exercises:

Instrumentation:

1. **Potentiometry**

   a. Acid-Base, Redox Titrations.

   b. Determination of stability constants of suitable complex systems.

2. **Conductometry**
   Acid-Base and precipitation Titrations

3. **Flame Photometry:**
   a. Estimation of sodium and potassium in admixture.
   b. Estimation of magnesium and calcium in tap water.
   c. Estimation of calcium in calcium salt solution.

CHE-540N: Research Projects* (Inorganic)

(0+4 Credits)

Project Titles:

1. Preparation and characterization of inorganic complex.
2. Spectrophotometry.

*Under the research project, the student can conduct experiments, engage in review writing, perform lab work, or complete dissertation work related to the syllabus of a particular semester, all under the supervision of the assigned mentor.

CHE-539N: Practical (Organic)

(0+4 Credits)

Marks (Practical): 100; Time: 8 h in two days;

Marks distribution (Practical)

Practical: 75 marks

Internal Assessment: 25 marks

Exercises:

1. Analysis of ternary organic mixture
2. Estimation of glucose.
3. Separation of organic mixtures by TLC method.

CHE-540N: Research Projects* (Organic)

(0+4 Credits)

Project Titles:

1. Identification and estimation methods of carbohydrate(s)
2. Synthesis and characterization of organic compounds

*Under the research project, the student can conduct experiments, engage in review writing, perform lab work, or complete dissertation work related to the syllabus of a particular semester, all under the supervision of the assigned mentor.

Open Elective Course (for other PG programmes)

CHE-541N: Chemical Techniques

(4+0 Credits)

Unit I

Sampling methods and lab practices

Methods of sampling solids, liquids and gases, good lab practices, lab safety, waste disposal and managements, methods of storing chemicals, solvents and glassware.

Unit II

Introduction to basic non-instrumental laboratory techniques

Sample preparation, solution preparation, gravimetric analysis and volumetric techniques such as complexometric titration and types of EDTA titration.

Unit III

Introduction to basic instrumental laboratory techniques

Use and maintenance of analytical balance, potentiometer, pH meters, conductivity meters, mechanical stirrers, melting point apparatus, water heaters, water deionisers, magnetic stirrers and hot plates etc.

Unit IV

Fundamental aspects of various spectroscopy techniques

Introduction to UV-Visible, IR, NMR, EPR spectroscopies and Magnetic Measurements.

Unit V

Fundamental aspects of some analytical techniques

Basic principle, instrumentation and applications of Chromatographic methods, Atomic absorption spectroscopy and Flame photometry.

Reference Books:

1. Willard, H.H., Merritt, L.L., Dean, J.A., Instrumental methods of analysis, CBS Publishers and distributers, Shahdara, Delhi, 1986.
2. Skoog, D., West, D., Principles of instrumental analysis, Cengage Learning, 2006.
3. Christian, G.D., Dasgupta, P.K., Schug, K.A., Analytical chemistry, Wiley India Pvt Ltd, 2012.
4. Vogel, A.I., Tatchell, A.R., Furnis, B.S., Hannaford, A.J., Smith, P.W.G. Vogel's practical organic chemistry, Pearson Education India, 1996.
5. Vogel, A.I., Elementary practical organic chemistry: Small scale preparations Part 1, Pearson Education India, 2010.
6. Silverstein, R. M., Webster, F.X., Spectrometric identification of organic compounds, John Wiley and Sons, 1997.

CHE-542N: Green Chemistry

(4+0 Credits)

Unit I

Introduction to Green Chemistry

What is Green Chemistry? Need for Green Chemistry. Goals of Green Chemistry. Limitations/ Obstacles in the pursuit of the goals of Green Chemistry

Unit II

Principles of Green Chemistry and Designing Chemical Synthesis

Principles of Green Chemistry with their explanations and special emphasis on the following with examples:

- Prevention of Waste/ byproducts
- Prevention/ minimization of hazardous
- Green solvents– super critical fluids, water as a solvent for organic reactions
- Energy requirements for reactions – alternative sources of energy: use of microwaves and ultrasonic energy

Unit III

Examples of Green Synthesis/ Reactions

- Green Synthesis of the following compounds: adipic acid, catechol
- Microwave assisted reactions in water: Hofmann Elimination, methyl benzoate to benzoic acid, oxidation of toluene and alcohols; microwave assisted reactions in organic solvents Diels-Alder reaction and Decarboxylation reaction
- Surfactants for Carbon Dioxide – replacing smog producing and ozone depleting solvents with CO_2 for precision cleaning and dry cleaning of garments.

Unit IV

Green Chemistry using Bio Catalytic Reactions

Introduction, Fermentation and Bio transformations, Production of Bulk chemicals by microbial fermentation

Unit V

Future Trends in Green Chemistry

Oxidation reagents and catalysts, Biomimetics, multifunctional reagents, Proliferation of solventless reactions, Green chemistry in sustainable development.

Reference Books:

- Ahluwalia, V.K. and Kidwai, M.R. New Trends in Green Chemistry, Anamalaya Publishers, 2005
- Anastas, P.T. and Warner, J.K. Oxford Green Chemistry -Theory and Practical, University Press, 1998

- Matlack, A.S. Introduction to Green Chemistry, Marcel Dekker, 2001
- Cann, M.C. and Connely, M.E. Real-World Cases in Green Chemistry, American Chemical Society, Washington, 2000
- Ryan, M.A. and Tinnesand, M., Introduction to Green Chemistry, American Chemical Society Washington, 2002
- Lancaster, Mike, Green Chemistry an Introductory Text 2 nd Ed., RSC Publishing,. ISBN: 978- 1-84755-873-2
- Dey, S. P. and Sepay, N., A Text Book of Green Chemistry, 1st Ed., Techno World, 2021

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