

# Jadavpur University

## M. Sc. Chemistry (CBCS) Syllabus

M. Sc. (CBCS) Course in Chemistry is a FOUR-SEMESTER curriculum.

### 1. Mode of Exercise of CHOICE by the student:

Two Theoretical papers will be allotted as Choice-based papers in the 3<sup>rd</sup> Semester.

Papers IX-IP-1 and IX-IP-2 along with Papers X-AO-1 and X-AO-2 are the Choice-based papers. Students will exercise their choice before the commencement of 3<sup>rd</sup> Semester in the following pattern:

a) **Any one** from IX-IP-1 and IX-IP-2 (Choice-based Papers)

Paper IX-IP-1: [Inorganic(1) + Physical(1)]; 4 Credits; Full Marks: 50

Paper IX-IP-2: [Inorganic(2) + Physical(2)]; 4 Credits; Full Marks: 50

b) **Any one** from X-AO-1 and X-AO-2 (Choice-based Papers)

Paper X-AO-1: [Analytical(1) + Organic(1)]; 4 Credits; Full Marks: 50

Paper X-AO-2: [Analytical(2) + Organic(2)]; 4 Credits; Full Marks: 50

### 2. Allocation of Special Paper:

3<sup>rd</sup> and 4<sup>th</sup> Semesters will be dedicated for Specialization. As usual, students will opt for Specialization from the following list before the commencement of 3<sup>rd</sup> Semester.

- a) Analytical Chemistry
- b) Inorganic Chemistry
- c) Organic Chemistry
- d) Physical Chemistry

### 3. Definition of Credit Points (CP) and Marks:

a) Theoretical Papers:

01 Credit  $\equiv$  One period (One hour duration) per week for 15 weeks

b) Practical Papers:

01 Credit  $\equiv$  Two periods (Two hours duration) per week for 15 weeks

## Distribution of Credit Points and Marks:

Semester	Paper	Unit	Credit per Unit	Marks per Unit	Total Credit for the Paper	Full Marks for the Paper	Grand Total for the Semester	
							Credit	Marks
I	I (Theoretical Chemistry)	1011	02	25	04	50	24	300
		1012	02	25				
	II (Organic Chemistry)	1021	02	25	04	50		
		1022	02	25				
	III (Inorganic Chemistry)	1031	02	25	04	50		
		1032	02	25				
	IV (Physical Chemistry)	1041	02	25	04	50		
		1042	02	25				
	L – I (Computer in Chemistry)	Parts I (Phy), II (Inorg), III(Org)			04	50		
	L – II (Organic Chemistry Practical)				04	50		
II	V (Biochemistry and Environmental Chemistry)	2051a	01	12.5	04	50	24	300
		2051b	01	12.5				
		2052a	01	12.5				
		2052b	01	12.5				
	VI (Organic Chemistry)	2061	02	25	04	50		
		2062	02	25				
	VII (Inorganic Chemistry)	2071	02	25	04	50		
		2072	02	25				
	VIII (Physical Chemistry)	2081	02	25	04	50		
		2082	02	25				
	L – III (Inorganic Chemistry Practical)				04	50		
	L – IV (Physical Chemistry Practical)				04	50		

**Distribution of Credit Points and Marks:**

Semester	Paper	Unit	Credit per Unit	Marks per Unit	Total Credit for the Paper	Full Marks for the Paper	Grand Total for the Semester	
							Credit	Marks
III	IX-IP-1 / IX-IP-2 (Choice-based paper)	309-I-1 / 309-I-2	02	25	04	50	24	300
		309-P-1 / 309-P-2	02	25				
	X-AO-1 / X-AO-2 (Choice-based paper)	310-A-1 / 310-A-2	02	25	04	50		
		310-O-1 / 310-O-2	02	25				
	XI-A / XI-I / XI-O / XI-P (Special Paper)	A / I / O / P-3111	02	25	04	50		
		A / I / O / P-3112	02	25				
	XII-A / XII-I / XII-O / XII-P (Special Paper)	A / I / O / P-3121	02	25	04	50		
		A / I / O / P-3122	02	25				
L-V-A / I / O / P (Special Practical)				04	50			
L-VI-A / I / O / P (Special Practical)				04	50			
IV	XIII-A / XIII-I / XIII-O / XIII-P (Special Paper)	A / I / O / P-4131	02	25	04	50	24	300
		A / I / O / P-4132	02	25				
	XIV-A / XIV-I / XIV-O / XIV-P (Special Paper)	A / I / O / P-4141	02	25	04	50		
		A / I / O / P-4142	02	25				
	XV-A / XV-I / XV-O / XV-P (Special Paper)	A / I / O / P-4151	02	25	04	50		
		A / I / O / P-4152	02	25				
	XVI-A / XVI-I / XVI-O / XVI-P (Special Paper)	A / I / O / P-4161	02	25	04	50		
		A / I / O / P-4162	02	25				
L-VII-A / I / O / P (Special Practical)				04	50			
L-VIII-A / I / O / P (Special Practical)				04	50			

**Total Credit Point for FOUR Semesters: 24+24+24+24=96**

**Full Marks for FOUR Semesters: 300+300+300+300=1200**

**Total Credit Point for Theoretical Papers in FOUR Semesters: 64**

**Total Credit Point for Practical Papers in FOUR Semesters: 32**

**Total Marks for Theoretical Papers in FOUR Semesters: 800**

**Total Marks for Practical Papers in FOUR Semesters: 400**

**Jadavpur University**  
**Two Year (4 Semester) PG-CBCS Syllabus in**  
**Chemistry**

**1<sup>st</sup> Semester**

**PAPER: I [Theoretical Chemistry]      CP (Credit Point): 4      Marks: 50**

**Unit-1011: Quantum Mechanics      (2L/W; CP: 2)      Marks: 25**

**Operators in Quantum Mechanics:** Linear and angular momentum operators and their commutation; step up–step down (ladder) operators. Creation and Annihilation operators.

**Basic formulations of Quantum Mechanics:** Postulates; Schrödinger equation; stationary and dynamic states; measurements in quantum mechanics; Heisenberg uncertainty relation (derivation of the general form); time-dependent Schrödinger equation; time variation of average values of Dynamical observables; Heisenberg equation of motion.

**Quantum mechanical study of selected model systems (stationary states):**

- (i) A particle in a circular path (Quantization of angular momentum).
- (ii) One-dimensional harmonic oscillator (Vibration of diatomic molecules the anharmonic terms).
- (iii) Three dimensional rigid rotator (Molecular motion, the centrifugal distortion).
- (iv) An electron in a central field potential (H-atom and H-like ions); their eigenfunctions and eigenvalues (derivation); properties of wave functions and related polynomials; calculation of average values of various physical observables of interest

and selection rules for transition (derivation for the above systems). In addition, alternative derivation of eigenvalues and eigenvectors of harmonic oscillator by ladder operator technique (creation and annihilation operators).

### **Electron Spin:**

Spin as an independent variable; experimental evidences, orbital and spin angular momentum; the magnetic moment ( $L+2S$ ); spin ladder operators; spin orbit coupling (Vector Model approach). Pauli Spin-matrices.

**Many electron systems:** the independent particle model; antisymmetry principle; the determinant (Slater) form of many electron wave function; the spin orbital; illustrative examples with He and Li atoms.

**Diatomic Molecules:** Separation of electronic and nuclear motion, MO treatment of  $H_2^+$ ; MO and VB treatment of  $H_2$ ; dissociation energy, two-centre integrals.

### **Unit– 1012 : Group Theory:**

**(2L/W; CP:2)**

**Marks: 25**

#### ***Groups and their representations:***

**(i)** Groups and their properties – the concept of groups; subgroups, cosets, classes and the related theorems; commutative (Abelian) groups, cyclic groups; isomorphism and homomorphism and their examples; group multiplication tables and the rearrangement theorem.

**(ii)** The point groups – symmetry elements and symmetry operations (recapitulation) of molecular species; point groups by symmetry operations; molecular point groups; stereographic projection; the matrix representations of symmetry operations; platonic solids.

#### ***Theory of group representations:***

**(i)** Mathematical recapitulation– unitary and hermitian matrices; similarity transformation and the invariance of characters; eigen values and matrix equations

under such transformations; block diagonalisation; direct product of matrices and their characters etc.

(ii) Representation theory – matrix representation of point groups; reducible, irreducible and equivalent representations; the Great Orthogonality Theorem (no derivation) and its corollaries; character tables, the row/column orthogonality of characters, construction of character tables in simple cases ( $C_{2v}$ ,  $C_{3v}$ ,  $T_d$  etc.); the basis functions, “projection” and “transfer”, operators (Bloch); reduction of a representation, the standard reduction formula; the direct product representation and its decomposition. Use of the projection operator to form symmetry adapted linear combination (SALC) of a simple system.

**PAPER: II [Organic Chemistry] CP: 4 Marks: 50**

**Unit– 1021 : Spectroscopy-I (2L/W; CP:2) Marks: 25**

NMR spectroscopy (theory, chemical shift, spin-spin splitting, strongly coupled systems, shift reagents, NOE [preliminary idea], Dynamic NMR [variable temperature], equilibrium study, difference between CW and FT-NMR,  $^{13}\text{C}$  NMR); Mass spectrometry (EI, CI, fragmentation of simple organic molecules); Structure elucidation of Organic molecules by Spectroscopic methods; Investigation of reaction mechanism by spectroscopic methods.

**Unit–1022 : Stereochemistry (2L/W; CP:2) Marks: 25**

Cyclohexene, allylic strains ( $A^{1,2}$ ,  $A^{1,3}$ ), cyclohexanone, alkyl ketone effect,  $\alpha$ -haloketone effect, effect of conformation on reactivity in acyclic compounds and cyclohexane, cyclohexene, cyclohexanone, polycyclic compounds (hydrindane, decalin, octalin, perhydroanthracene and perhydrophenanthrene), Conformations of piperidine and tetrahydropyran, decahydroquinoline and quinolizidine. Dynamic stereochemistry. Chiroptic properties (circular birefringence and circular dichroism), Cotton effect, Axial haloketone rule, Octant rule.

<b>Paper: III [Inorganic Chemistry]</b>	<b>CP: 4</b>	<b>Marks: 50</b>
<b><u>Unit-1031</u></b>	<b>CP: 2</b>	<b>Marks: 25</b>
<b><u>1031a: Theories of the electronic structure of transition metal complexes</u></b>		
	<b>(1L/W; CP:1)</b>	<b>Marks: 12.5</b>

***Adjusted C.F. Theory (the Ligand Field Theory):***

- (i) Recapitulation of basic concepts.
- (ii) Spin-orbit coupling constant and interelectronic repulsion parameters in complex ion terms-vs-free ion terms, Nephelauxetic effect. Adjusted crystal field theory.
- (iii) Interpretation of the general features of the electronic absorption spectra, including the charge transfer spectra of the transition metal complexes in aqueous solutions.

***Qualitative M.O. treatment:***

MO energy diagram for octahedral ML<sub>6</sub>, tetrahedral ML<sub>4</sub> and square planar ML<sub>4</sub> complexes with sigma-only donor ligands; MO energy diagram for octahedral ML<sub>6</sub> and tetrahedral ML<sub>4</sub> complexes with pi donor/ pi-acceptor ligands.

**1031b : Organometallic Chemistry (1L/W; CP:1) Marks: 12.5**

1. Application of 18-electron rule.
2. Organometallic compounds of non-transition elements-Al, Si and Hg: preparation, properties and reactions: structure and bonding and applications. Special aspects of Li and Mg.
3. Metal-carbon-bonded compounds (compounds of the sigma electron ligands). Homoleptic and heteroleptic compounds: synthesis, reactivity, oxidative addition and reductive elimination reaction: insertion reactions; Metallacycles.
4. Five electron ligands  $\eta^5$ -complexes of cyclopentadiene and substituted cyclopentadienes-both sandwich [bis(cyclopentadienyl)metal complexes] and half sandwich types of complexes; Multidecker sandwich compounds. Metal arene complexes:  $\eta^6$  mode,  $\eta^4$  mode and  $\eta^2$  mode of binding; bis-arene complexes:

synthesis, structure and reactivity; half-sandwich arene complexes including piano-stool complexes: selected examples, their synthesis and structure.

**Unit-1032**

**CP: 2**

**Marks: 25**

**1032a: Inorganic reaction mechanism-I (1L/W; CP:1)**

**Marks: 12.5**

***Substitution reaction:***

**(i)** Stability and reactivity, Interpretation of Mechanistic labels - A, D, I, I<sub>a</sub>, I<sub>d</sub>; comparison with S<sub>N</sub>1, S<sub>N</sub>2, Intimate Mechanism and Stoichiometric Mechanism.

**(ii)** Tools of the trade: Rate law, activation parameters, principle of microscopic reversibility, etc.

Derivation of rate laws for complex systems and analyses of such rate laws.

**(iii)** Studies on Octahedral complexes of Fe(II)/Fe(III), Co(III), Cr(III), Rh(III): aquation, anation, pseudosubstitution acid catalysed aquation, base hydrolysis, Isomerisation and racemisation reaction: the Ray-Dutta twist and Bailier twist mechanism: Square planar complexes of Pt(II); trans-effect in substitution reactions.

**1032b: Nuclear Chemistry**

**(1L/W; CP:1)**

**Marks: 12.5**

1. Nuclear Shell model. Determination of spin parity. Stability of Super heavy elements.
2. Artificial Nuclear Reactions: Various important nuclear reactions, Bethe's notation of nuclear reactions, Nuclear reactions versus chemical reactions, Classification of nuclear reactions, Szilard-Chalmer's effect and its uses.
3. Nuclear Fission: Spontaneous fission, Mechanism of nuclear fission, Chain reactions of fissions, Atom bomb, Nuclear reactor, Breeder Reactor, neutron economy, four factor formula.
4. Radiochemical Methods of Analysis: Neutron activation analysis, isotopic dilution analysis, Analysis related with biological, medical and agriculture fields, Determination of structures and establishment of reaction mechanisms.

**PAPER: IV [Physical Chemistry] CP: 4 Marks: 50**

**Unit– 1041: Chemical Thermodynamics (2L/W; CP:2) Marks: 25**

1. Brief resume of the concept of entropy, free energy and laws of Thermodynamics and general conditions of Equilibria.
2. Thermodynamic properties (fugacity & fugacity coefficient) of gases with special reference to real gases in the pure state and in mixtures.
3. Mixture (reacting and non-reacting) system: Gibbs Duhem equations; partial molar quantities, their significances and methods of determination. Dependence of different partial molar quantities on composition.
4. Binary solution: Raoult and Henry laws; Chemical potential of the components of ideal and non-ideal solutions, excess functions (activity coefficient and osmotic coefficient) for non-ideal solutions and their determination. Different scales of activity and activity coefficients for solutes and solvents. Experimental determination of activity coefficients of electrolytes and non-electrolytes.
5. **Ion–Ion Interactions:** Debye-Huckel ionic atmosphere theory, Limiting & Extended Debye Huckel Equations for activity coefficient. Test of the Theory; Robinson and Stokes equations for activity coefficient.

**Unit– 1042: Electrochemistry (2L/W; CP:2) Marks: 25**

**Ion Solvent interactions:** Concept, experimental determination, application to equilibria, kinetics, universal scales of potential acidity and basicity in different solvents. Born Model & Eley-Evans model, Absolute heats of hydration (Halliwell&Nyburg Method).Solvation number and its determination. Ion-solvent-non-electrolyte interactions: Salting-in and salting-out phenomena.

**Ion-Association:** Bjerrum and Fuoss equation for ion-pair formation. Conductance minima, Ion-triplet, Ion-quadruplets; Walden's empirical rule and Fuoss treatment of

conductance minima. Fuoss Shedlovsky's method of determination of association constant.

**Ion-transport in solution:** Fick laws and equations of Einstein on diffusion, Limiting Debye Huckel-Onsager Expression. (Electrophoretic effect, Relaxation effect and time of relaxation). Transport number as a function of concentration. Wien Effect, Debye-Falkenhagen effect, Nernst Hartley Expression, Viscosity B-Coefficients.

**PAPER: L-I [Computer in Chemistry] (8L[2days]/W; CP : 4) Marks: 50**

### **Part-I (Physical Chemistry; 10 Days)**

1. Introduction to Computers & Linux Operating System
2. Introduction to FORTRAN-77 Language
3. Numerical analysis with Fortran Programming:
  - (a) Sorting and Ordering; (b) Matrix addition, multiplication; (c) Introduction to concepts of accuracy, precession, error, standard deviation and correlation coefficients; (d) Least square fitting of curves.

### **Part-II (Inorganic Chemistry; 10 Days)**

Scope of Computational Chemistry, Concept of Basis Set and Correlation Functional; Geometry optimization and semi-empirical calculations (NH<sub>3</sub>, H<sub>2</sub>O, CO, NO etc.); Calculation of bond energy, formation energy, ionization potential etc. (Model systems); Concept and construction of molecular orbitals.

### **Part-III (Organic Chemistry; 10 Days)**

#### **a) Chemical design:**

(i) Drawing of chemical structures, captions and atom labels, orbitals, symbols, and other shapes, (ii) Manipulating drawings, (iii) Drawing query structures.

#### **b) Reactions and synthesis:**

(i) Discovery of catalytic pathways, (ii) Improvement of isomer ratios and synthesis yields.

**c) Drug discovery:**

(i) Automatic conversion of 2D structures to 3D, (ii) Descriptors availability, (iii) QSAR/QSPR studies.

**d) Stereochemical Analysis:**

Conformational analysis of simple organic molecules, di and tripeptides using molecular mechanics calculation.

**Paper: L-II [Organic Chemistry Practical] (8L[2days]/W; CP: 4) Marks : 50**

1. Identification of organic compounds by systematic qualitative and spectroscopic analyses.
2. Estimation of nitrogen by Kjeldahl method / estimation of methoxy group by Ziesel method.
3. Preparation of some useful organic compounds.

**2<sup>nd</sup> Semester****Paper: V [Biochemistry & Environmental Chemistry] CP: 4 Marks : 50****Unit– 2051a: Bioinorganic Chemistry (1L/W; CP: 1) Marks: 12.5**

Introduction to Metallobiomolecules. Metal ions in some basic reactions in biological systems. (a) The bioinorganic aspect related to oxygen in O<sub>2</sub> transport by the combination of Hemoglobin and Myoglobin; hemerythrin, hemocyanin (b) N<sub>2</sub> fixation (Nitrogenase); (c) Metals and diseases; (d) Chelation therapy - role of different chelating agents in the removal of in vivo metal overload.

**Unit– 2051b : Environmental Chemistry (1L/W; CP: 1) Marks: 12.5**

Introduction to environmental chemistry and its classification; Gaseous pollution – inter-relation between organic, inorganic, physical and analytical chemistry. Toxic inorganic substances – realizing toxicity from the SHAB standpoint. Health hazards of

SPM [Suspended (inorganic) Particulate Matter]; IPM [Inhaleable (inorganic) Particulate Matter]; Methods of determination of SPM (High Volume Sampler) and IPM (Cascade Impactor); Mechanisms of some heavy metal toxicities and their impact on society; Pesticides; metallo-organic compounds and their toxicity; Application of analytical methods to determine toxic species.

**Unit– 2052a: Bioorganic Chemistry (1L /W; CP: 1) Marks: 12.5**

**1. Enzymes:** Classification, function, enzyme models, kinetics of enzymatic catalysis, serine and cysteine proteases, co-factors, co-enzymes and metalloproteins, Baker's yeast.

**2. Metabolism:** Primary and secondary metabolites, their importance and biosynthesis. *Carbohydrate metabolism:* Glycolysis, TCA-cycle, Glycogen biosynthesis, Glycogenolysis, Reactions of Gluconeogenesis, Cori Cycle, Comparison between Gluconeogenesis and glycolysis *Amino acid Metabolism:* Oxidative deamination, Transamination, Decarboxylation, Transmethylation, Urea cycle, *Fatty acid metabolism:*  $\beta$ -oxidation.

**Unit– 2052b: Surface & Biophysical Chemistry (1L/W; CP:1) Marks: 12.5**

**Mobile interface:** Orientation at interfaces, spreading of films, applications.

**Immobile interface:** Multilayer adsorption (BET and Harkins Jura Theory) Thermodynamics, Hysteresis.

**Association Colloids:** Micelles, Microemulsion formation, Thermodynamics, Application (detergency).

**Biophysical:** Introduction to structure and function of Proteins and Nucleic acids and their stability.

**Paper: VI [Organic Chemistry] CP: 4 Marks: 50**

**Unit–2061: Pericyclic Reactions, Photochemistry, Reaction Mechanism & Synthetic Methodologies (2L/W; CP: 2) Marks: 25**

Electrocyclic, cycloaddition, sigmatropic reactions (FMO Theory, correlation diagrams), Linear Free Energy Relationship, HSAB principle, Basic Principles of organic

photochemistry (Franck-Condon principle, Jablonski diagram, singlet and triplet states, Norrish Type I and II processes), Reducing agents (nucleophilic, electrophilic, single electron transfer), oxidizing agents.

### **Unit-2062 : Heterocyclic Chemistry & Natural Products**

**(2L/W; CP: 2)      Marks: 25**

Chemistry of heterocyclic compounds containing two heteroatoms in a ring – Reactions of diazines and purines with emphasis to nucleophilic substitution and Dimroth rearrangement; reactions of azoles with reference to N-heterocyclic carbenes along with their applications in organic synthesis and biology; synthesis of azole, azine and purine ring systems through the syntheses of some compounds of pharmaceutical importance (e.g. carbaBVDU, trimethoprim, metronidazole, adenosine, sildenafil, aciclovir, allopurinol etc.); a few examples of organic transformations with temporary construction of heterocyclic systems as intermediates.

Chemistry of monoterpenoids (geraniol, menthol, pinenes, camphor); alkaloids (nicotine, ephedrine, atropine); coumarins and flavonoids. Preliminary idea of biosynthesis of these classes of natural products.

**Paper: VII [Inorganic Chemistry]      CP: 4      Marks : 50**

**Unit-2071      CP: 2      Marks: 25**

**2071a : Metal Cluster & Boranes      (1L/W; CP:1)      Marks: 12.5**

#### ***Metal Cluster:***

Introduction, Cluster compounds of heavier transition elements in particular, their halides and carbonyls including the bridged carbonyl, their preparation, properties and structures (inorganic rings, cages, Keggin and clusters), Zintl ions.

Metal-metal bonds in the metal atom cluster compounds (including quadrupole bond in binuclear complexes). Experimental evidence of existence of such bonds.

Bonding in metal atom cluster – qualitative M.O. theory including Hoffmann's isolobal concept.

#### ***Boranes:***

Boron hydrides (Boranes) – Structure, bonding and Lipscomb's topology; 'styx' system of numbering; Nomenclature.

Carboranes, Metalloboranes and Metallocarboranes– Synthesis and structure; Wade's rules, Jemmis concept.

Boron compound of potential medicinal interest; Boron neutron capture therapy (BNCT).

### **2071b : Chemistry of the Platinum Group Metals**

**(1L/W; CP:1)**

**Marks: 12.5**

1. Platinum Group Metals: oxidation state, valence preference toward  $\pi$ -donor and  $\pi$ -acceptor ligands.
2. Cyclometalated complexes. Chemistry of Platinum Group Metals with redox non-innocent ligands: radical complexes. Dinitrogen complexes. Chemistry of dioxygen complexes. Dihydrogen complexes. Nitrosyl complexes of ruthenium in the perspective of structure and bonding.
3. Some historically important compounds: Creutz-Taube compound, Vaska's compound, Magnus' green salt, Vauquelin's pink salt, Krogmann salt etc.

### **Unit-2072**

**CP: 2**

**Marks: 25**

#### **2072a : Diffraction methods and ESR spectroscopy**

**(1L/W; CP:1)**

**Marks: 12.5**

1. General idea of electron, neutron and X-ray diffractions.
2. E.S.R spectroscopy: General background of E.S.R spectroscopy; representation of ESR spectrum, g value, E.S.R spectra of simple organic free radicals and related species; hyperfine coupling; prediction of expected number of lines and their relative intensities, hyperfine splitting in various systems, factors affecting the magnitude of g-value; zero-field splitting and Kramers' degeneracy. Applications.

**2072b : Theory and Application of some Analytical Techniques in Chemistry****(1L/W; CP:1)****Marks: 12.5*****Solvent extraction:*** Brief recapitulation and use of different organic reagents.***Chromatography:*** General Principle, classification, mathematical relations of capacity, distribution constant and retention time; chromatogram; band broadening and column efficiency; column resolution, paper chromatography, TLC, size-exclusion chromatography, ion-exchange chromatography: ion exchange capacity and its determination. Capillary electrophoresis.***Metal-chelates in solution:*** Determination of stability constants. Kelvin- Bjerrum method for determination of stability of complexes. Stability of ternary complexes – importance in biology.**PAPER: VIII [Physical Chemistry]****CP: 4****Marks: 50****Unit– 2081: Chemical Kinetics****(2L/W; CP:2)****Marks: 25**

Theory of reaction rates: Hard sphere collision theory & its limitation, Unimolecular reaction & Lindeman theory, Potential energy curves and surfaces, Conventional transition state theory (CTST), Thermodynamic formulation of CTST, Applications of CTST (reactions between atoms and molecules, unimolecular reactions, ter/trimolecular reactions), Limitations of CTST, Comparison between collision and transition state theory; Thermodynamic treatment of reaction rates, Energy of activation, Volume of activation; Determination of rate constant of fast reactions, Basic principles of fast kinetics, Flow and stopped flow techniques, Relaxation methods, Flash photolysis; Chain reactions and chain length; Effects of isotope (equilibrium and kinetic), solvent, and dielectric constant on reaction rate, Effect of ionic strength on reaction rate & derivation of Brönsted-Bjerrum equation; Effect of substituents, Linear free energy relationship, Hammett's and Taft's constants, Hammett's acidity function; Mechanism of specific and general acid-base catalysis.

**Unit– 2082: Statistical Mechanics****(2L/W; CP:2)****Marks: 25**

1. Mathematical and thermodynamic probability-concept of ensemble and postulates of statistical mechanics, Microcanonical, canonical and grand canonical ensembles –

most probable distribution, independent subsystems and distinguishability – classical partition function-phase space – Liouville's theorem-Ergodic hypothesis.

2. Thermodynamic parameters and function for different ensembles – fluctuation in thermodynamic quantities - statistical interpretation of classical thermodynamics – (including laws of thermodynamics, equipartition of energy principle, residual entropy).

3. A brief review of translational, rotational, vibrational and electronic modes of motion for ideal gases. Related thermodynamic quantities. Equilibrium constant in terms of partition functions.

4. Heat capacity of solids – Einstein and Debye treatment.

5. Adsorption – Langmuir and BET isotherm.

6. Preliminary idea of Quantum Statistics, Indistinguishable and distinguishable particles, Derivation of FD and BE Statistics.

**Paper: L-III [Inorganic Chemistry Practical] (8L[2days]/W;CP: 4) Marks : 50**

**1. Analysis & estimation**

(a) Gravimetric Analysis of Ni in Ni-Steel.

(b) Studies on the composition of complexes by Job's, Mole ratio and Slope ratio methods.

(c) Estimation of ascorbic acid in commercially available tablets.

**2. Preparation and characterization of 3d metal compounds:**

Schiff base complexes, Reinecke's Salt,  $[\text{Ni}(\text{en})_3]\text{Cl}_2$ ,  $[\text{VO}(\text{acac})_2]$ ,  $[\text{Co}(\text{NH}_3)_5(\text{ONO})]\text{Cl}_2$ ,  $[\text{Co}(\text{NH}_3)_5(\text{NO}_2)]\text{Cl}_2$  etc.

**Paper: L-IV [Physical Chemistry Practical] (8L[2days]/W; CP: 4) Marks: 50**

1. Determination of thermodynamic solubility product of a sparingly soluble salt in aqueous medium.

2. Determination of the enthalpy of solution of a sparingly soluble monobasic acid by solubility measurements.

3. Determination of critical solution temperature of phenol-water system in presence of 5 & 10 % NaCl

4. Determination of average relative molecular mass of a polymer viscometrically

5. Determination of rate constant and order of the reaction:  $\text{KBrO}_3 + 5\text{KBr} + 6\text{HCl} \rightarrow 6\text{KCl} + \text{Br}_2 + 3\text{H}_2\text{O}$ ; titrimetrically
6. Determination of strength of NaOH solution by standard oxalic acid solution conductometrically
7. Determination of individual strength of  $\text{Na}_2\text{SO}_4$  and  $(\text{NH}_4)_2\text{SO}_4$  in their mixture conductometrically
8. Determination of rate constant of acid catalyzed mutarotation of  $\alpha$ -D-glucose at different acid concentrations polarimetrically
9. Study the effect of ionic strength on the reaction:  $\text{K}_2\text{S}_2\text{O}_8 + \text{KI} \rightarrow 2\text{K}_2\text{SO}_4 + \text{I}_2$ ; spectrophotometrically.
10. Determination of individual strengths of KCl, KBr & KI in a solution of their mixture potentiometrically.
11. Determination of the redox potential  $E^0$  of the quinhydrone electrode potentiometrically.
12. Determination of individual strength of HCl and AcOH in their mixture pH-metrically
13. Determination of CMC and spreading coefficient of surfactants from surface tension measurements.
14. Determination of the Zeta potential of a colloid by electrophoresis.

### 3<sup>rd</sup> Semester

#### CHOICE-BASED PAPERS

Two Theoretical papers (any one from the Papers IX-IP-1 and IX-IP-2 along with any one from the Papers X-AO-1 and X-AO-2) are the Choice-Based Papers.

**PAPER: IX-IP-1                      CP: 4                      Marks: 50**

**Unit-309-I-1: [Inorganic Chemistry (I<sub>1</sub>)]                      CP: 2                      Marks: 25**

**309-I-1a: Inorganic Solid Materials                      (1L/W; CP:1)                      Marks: 12.5**

1. Preparative methods of Solids: Solid state reaction, Crystallization of solutions, Vapour phase transport methods, Ion exchange and Intercalation methods,

Electrochemical reduction methods, Growth of single crystals, High pressure and hydrothermal methods.

2. Inorganic Descriptive Crystal Chemistry: Structures with respect to Metals, Alloys, Ionic and Covalent Network Structures, Molecular Structures. Pauling rules for understanding of structures, Mechanisms and impacts on properties due to crystal defects and non-stoichiometry of inorganic solids.

3. Structure of Network solids: Concept of node, Ring and Circuit, Nomenclature of networks, Wells Notation, Schläfli Symbol, Vertex Symbol.

4. Role of Structures on the Properties of Inorganic Solid Materials: Optical, Magnetic and other related properties.

**309-I-1b: Inorganic Crystal Engineering (ICE) and Principle of Designing Porous Materials** (1L/W; CP:1) Marks: 12.5

1. Inorganic crystal engineering and design principle of metal-organic frameworks and organic-inorganic hybrids.

2. Principles of ICE in the design of porous materials, their understanding and characterizations using X-ray diffraction and thermal methods. Surface characterization and surface behavior of such porous materials with special reference to the gas/solvent vapors sorption.

3. Some special applications of such materials like gas storage, gas/solvent separation etc.

4. Understanding of the structure-property relationship for the design of functional molecular material or molecular devices- philosophy and the terminologies.

**Unit-309-P-1: [Physical Chemistry (P<sub>1</sub>)]** (2L/W; CP: 2) Marks: 25

**Macromolecules and Materials Chemistry**

**Macromolecules (including Polyelectrolytes):** Polymer conformation and chain dimension; Interaction with solvent, Thermodynamics of Polymer solution, Determination of interaction parameters, Donnan effect, pH difference across the

membrane, Membrane polarization and membrane potential, Molecular weight distribution and molecular weight average; Determination of molecular weight, size and shape by Membrane osmometry, vapour pressure osmometry, light scattering (Zimm method and Dissymmetry method), diffusion and Gel-permeation chromatography; viscosity of polymer solution.

**PAPER: IX-IP-2** **CP: 4** **Marks: 50**

**Unit-309-I-2: [Inorganic Chemistry (I<sub>2</sub>)]** **CP: 2** **Marks: 25**

**309-I-2a: Comparative Chemistry of d & f Block Elements**

**(1L/W; CP: 1) Marks: 12.5**

1. Electronic configuration, chemistry in different oxidation states and comparative study
2. Extraction of lanthanides from pitchblende, lanthanide separation, purification of plutonium-239
3. Properties and structures of the lower halides of Nb-Ta: Mo-W; Tc-Re with special emphasis on the metal atom clusters present.
4. Polyoxometallates, blue oxides of Mo-W, the tungsten bronze, sulphides of Mo.
5. Spectral and magnetic properties of d and f-block compounds and comparative study
6. Lanthanide Shift reagents and uses of lanthanide compounds

**309-I-2b: Supramolecular Chemistry** **(1L /W; CP:1) Marks: 12.5**

1. Origin of supramolecular chemistry
2. Nature and types of supramolecular interactions (Hydrogen bonding, van der Waal interactions,  $\pi$ -stacking, C-H... $\pi$  interactions, hydrophobic effects, solvation, etc.)
3. Concepts and terminology of supramolecular chemistry—Cooperativity, chelate effect, macrocyclic effect, Preorganisation and complementarity,

4. Molecular recognition- Different types of receptors with special reference of Crown ethers, Podands, cryptands, spherands; Synthesis of cryptands- template effect, high dilution synthesis
5. Anion recognition: challenges in anion receptor chemistry, host design for anion; anion coordination chemistry.
6. Self-assembly- formation and examples.
7. Application of supramolecular chemistry.

**Unit-309-P-2: [Physical Chemistry (P<sub>2</sub>)]      (2L/W; CP: 2)      Marks: 25**

**Nanomaterials:**

Introduction, Basic concept of nanoparticles, quantum dot; Synthesis: Chemical, solvothermal, electrochemical, photochemical, biophysical etc; Use of bacteria, fungi, ion beam etc; Stabilization of nanoparticle in solution; Characterization by TEM, SEM, AFM, DLS etc.; Properties: Electrical, Magnetic, optical and catalytic, role of size; Application of nanomaterials in different fields. Nanocomposite; Carbon nanotubes: synthesis, properties, applications and uses; Uses of nanomaterials. Conducting polymers and organic metals; Liquid crystals.

**PAPER: X-AO-1      CP: 4      Marks: 50**

**Unit-310-A-1: [Analytical Chemistry (A<sub>1</sub>)]      CP: 2      Marks: 25**

**310A-1a: Basic Characterization of Solid Materials:**

**(1L/W; CP:1)      Marks: 12.5**

1. Nature of solid; color and physical state of materials for predicting the mode of characterization. Destructive and non-destructive analysis of solids, their comparative advantages and disadvantages.
2. Importance of X-ray in the analysis of solids. Bragg's law and X-ray diffraction. Powder diffraction and Single crystal diffraction, their comparative ease and limitations.

Samples for powder X-ray diffraction (PXRD), experiment, and interpretation of data. Indexing of PXRD data and introductory idea about the database of known PXRD.

3. Introduction to thermal analysis: Thermogravimetric analysis (TGA), Differential thermogravimetric analysis (DTG), Differential thermal analysis (DTA) – Principles and methods, presentation of thermal data. Standard TG-DTA curve analysis ( $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$ ). Differential Scanning Calorimetry (DSC): comparative discussion of DSC with DTA. Applications of thermal methods of analysis with special reference to solid state reactions, decomposition of inorganic and organic solids. Stability of different compounds (with special emphasis to the inorganic porous compounds) and coupling of TG-PXRD technique. Desolvation / deaquation of inorganic / coordinated compounds, phase transition.

### **310A-1b: Microscopic Characterization of solid materials**

(1L/W; CP:1)

Marks: 12.5

1. Basic principles of image formation in electronic optics. Electron microscopy technique and its comparison with optical microscopy/light microscope. Applications of electron microscopy in the field of material science, forensic science and bioscience.
2. Sample preparation/mounting for the electron microscope: Different types of grid and choice of grids depending on the sample as well as techniques.
3. Different types of electron microscopy e.g. SEM/FESEM, TEM/HRTEM, EDX with their description, operational principle and application for analysis of different samples.

### **Unit-310-O-1: [Organic Chemistry (O<sub>1</sub>)]**

(2L/W; CP: 2)

Marks: 25

#### **Reagents and Name Reactions**

Mitsunobu reaction, Julia olefination, TEMPO-mediated reactions, Click chemistry, Staudinger reaction and ligation, Wittig/ Steven rearrangement, Neber rearrangement, multicomponent reactions (Biginelli reaction, Ugi reaction, Petasis reaction etc.) Prins reaction, Ohira-Bestmann reaction, Appel reaction, Corey-Fuchs reaction, Bergman cyclization, Eschenmoser reaction, Wacker oxidation, Grieco oxidation, Ito oxidation. Organoboranes in organic synthesis. Electrophilic and nucleophilic selenium reagents and their applications in organic synthesis.

**PAPER: X-AO-2****CP: 4****Marks: 50****Unit-310-A-2 [Analytical Chemistry (A<sub>2</sub>)] CP: 2 Marks: 25****310-A-2a: Mass Spectroscopy (1L/W; CP:1) Marks: 12.5**

Generation of ions and detection; EI and fragmentation pattern in EI; CI FD, FAB, plasma desorption etc. Analytical applications. GC-MS and its uses. Electron probe micro analysis (EPMA) and Laser Micro Probe Mass Analyzer (LAMMA): Theory and working principle, application with special reference to environmental analysis.

**310-A-2b: Photoelectron Spectroscopy (1L/W; CP:1) Marks: 12.5**

Photoelectron spectroscopy: photoexcitation and photoionization, core level (XPS) and valence level (UPS) photoelectron spectroscopy, XPS and UPS experiment, chemical shift, detection of atoms in molecules and differentiation of same element in different environments from XPS, information about the nature of molecular orbital from UPS, UPS of simple diatomic molecules, e. g., N<sub>2</sub>, O<sub>2</sub>, CO, HCl, etc.

**Unit-310-O-2: [Organic Chemistry (O<sub>2</sub>)] (2L/W; CP: 2) Marks: 25****Structure Activity Relationship, Hückel Calculations**

MO treatment of acyclic and cyclic conjugated systems, Hückel Molecular Orbital Theory (HMOT)– applications to ethylene, allyl, cyclopropenyl, butadiene, cyclobutadiene, pentadienyl, cyclo pentadienyl, hexatriene, Benzene, fulvene; Systems Involving Heteroatoms, Extended Hückel Theory (EHT), alternant and non-alternant hydrocarbons, Symmetry and Symmetry Operations in MOT, Group Orbitals, The Walsh Diagram: Planar and Pyramidal Methyl, The Walsh diagram for CH<sub>2</sub>, Orbital Mixing, Orbital mixing to construct Ethane and Ethylene, The Cyclic Three-Orbital Mixing, Walsh MO of Cyclopropane, Through-bond coupling in planar cyclohexadiene, MO of Carbenes; TASO, MO of methane, The Effects of Heteroatoms, Cieplak model.

## SPECIAL PAPERS

### Theoretical Papers

**Paper: XI-A [Analytical Chemistry Special] CP: 4 Marks : 50**

**Unit– A-3111 : Electroanalytical Methods (2L/W; CP:2) Marks: 25**

Electrochemical cell, electrodes, membrane electrodes, ion selective, molecular selective, gas sensing probes.

***Polarography:*** Basic principles – polarized depolarized electrodes; diffusion currents, DME, polarographic wave; Ilkovic equation (simplified derivation) and its significance; half wave potential, and its applications in identification of elements. Ilkovic-Heyrovsky Equation, Cottrell Equation. Stripping voltammetry, Amperometric titration. Modern developments in polarographic techniques; Lingane's method.

***Cyclic voltammetry, DPV and coulometry:*** Basic principles, three electrode system, reversible, quasireversible, irreversible cyclic voltammograms; Differential Pulse Voltammetry (DPV); R. S. Equation; electrosynthesis, electrocatalysis, electropolymerisation, Spectroelectrochemistry, Surface modrams. EC, ECE etc path ways, protic-electroprotic equilibria. Redox isomers, spatially isolated orbitals. Chronoamperometry, chronopotentiometry, photoelectrochemical solar cell (PEC).

**Unit– A-3112 : Fundamental and Instrumental aspects of Single crystal X-ray diffraction Technique (2L/W; CP:2) Marks: 25**

Concepts of crystal structure-Bravais lattice, crystal systems, indexing of lattice planes, translational and rotational symmetry, symmetry elements and their symbols (both numerical and graphical), point group, screw axis, glide plane, HM notation, space groups, centrosymmetric and non-centrosymmetric space groups, space group number and tables (few examples), equivalent position, Braggs law of diffraction, Reciprocal lattice and its relation with direct lattice, Ewald sphere, Different methods of diffraction (Laue, rotating crystal and powder), crystal growth (in brief), crystal mounting techniques using goniometer, centering of crystal, intensity of scattered

radiation, structure factor, data collection methods and strategy, data processing, different methods structure solution (direct, Patterson, intrinsic) and refinement, absorption correction, disorder problem, structure validation and publication, intro about CSD database and how to use it. Brief introduction of advanced techniques like Synchrotron X-ray radiation source.

**Paper: XI-I [Inorganic Chemistry Special] CP: 4 Marks : 50**

**Unit– I-3111 : X-ray Crystallography (2L/W; CP:2) Marks: 25**

Crystalline solid –single crystal and polycrystal (twining problem); lattice; unit cell – primitive and non-primitive unit cells, Unit cell parameters and crystal systems

X-ray, Generation of X-ray, Cu  $K\alpha$  and Mo  $K\alpha$  radiation; X-ray diffraction; Bragg equation;

Crystal symmetry – (i) point group elements and (ii) space group elements; 32 crystal classes, HM notations, distribution in different systems and stereographic projections; Isogonal symmetry groups

Space group – HM notation, space groups in triclinic and monoclinic systems

Indexing of lattice planes; Miller indices

Reciprocal lattice and its relation to direct lattice; Bragg reflection in terms of reciprocal lattice – sphere of reflection and limiting sphere; relation between  $d_{hkl}$  and lattice parameters.

Methods of growing single crystals; crystal mounting; data collection; structure solution; structure refinement; significance of R value; non-covalent interactions and its importance

Absorption correction; disorder problems.

**Unit– I-3112 : IR, Raman, CD and ORD Spectroscopy**

**(2L/W; CP:2)**

**Marks: 25**

Origin, absorption of radiation by molecular vibrations in polyatomic molecules, effects giving rise to absorption bands, group vibration, limitation of the concept, FTIR, NDIR techniques.

**Raman Spectroscopy:** Theory, instrumentation, mechanism of Raman Effect, effect in solids, liquids and gases, Use of symmetry considerations to determine the number of active infrared and Raman lines, differences of IR and Raman spectra, Laser Raman spectra application.

The symmetry origin of the optical activity of molecules, the phenomena of Optical Rotatory Dispersion (ORD) and Circular Dichroism (CD), the Cotton effect, application

**CD and ORD spectrometry:** principle, methodology and applications.

**Paper: XI-O [Organic Chemistry Special] CP: 4 Marks: 50**

**Unit– O-3111 : Pericyclic Reactions and Biosynthesis of Natural Products**

**(2L/W; CP:2) Marks: 25**

1. Electrocyclic reactions for  $4r$  &  $(4q+2)$ -electron systems along with state correlation diagrams with varied examples, based on symmetry considerations, Cycloaddition reactions for  $4r$  &  $(4q+2)$ -electron systems with state correlation diagrams based on symmetry analysis. Principles, Klopman-Salem equation & its application in chemical Reactions. Ionic cycloaddition reactions, Asymmetric Diels-Alder reactions, Regioselectivity, Periselectivity, Site selectivity, Stereoselectivity for  $4r$  &  $(4q+2)$ -electron systems.

Sigmatropic Reactions with FMO & modified FMO theory applications,  $[i, j]$ -shift highlighting  $[3,3]$ ,  $[2,3]$ ,  $[3,4]$  etc. shifts along with chiral substrates. Aromatic transition state theory.

2. Cheletropic Reactions involving neutral molecules & reactive species.

3. Ene Reaction, Prismane, Basketene, Barrelene, Bullvalene systems & their reactivities.

4. Pericyclic reactions in biological system.

5. Biosynthesis of primary and secondary metabolites: terpenoids (Lupeol, Taraxasterol,  $\alpha$ -Amyrin,  $\beta$ -Amyrin, Friedlane, Gibberellic acid), steroids (Cholesterol, Lanosterol etc.) and alkaloids (vincoside, Ajmalicine, Catharanthine, Cinchona alkaloids like quinine etc.).

**Unit– O-3112 : Photochemistry and Synthesis of Steroids****(2L/W; CP:2)****Marks: 25**

1. Photo-induced reactivity of olefins, *cis-trans* –isomerisation, Photochemistry of vision, Paterno-Buchi reaction, Photochemistry of ketones, unsaturated ketones and various conjugated systems, Lumiketone rearrangement, di- $\pi$ -methane rearrangement (DPM), Oxa-di- $\pi$ -methane (ODPM) aza-di- $\pi$ -methane (ADPM), Barton reaction, Hofmann-Loeffler-Freytag reaction, Photochemistry of arenes,  $S_{RN}1$ ,  $S_{RN}2$  and related reaction mechanisms, Photo-oxidation, photoreduction, photochemistry of imines and enamides and application in natural product syntheses, Visible light photocatalysis in organic syntheses.
2. Total synthesis of steroids and steroidal hormones (cholesterol, testosterone, progesterone, aldosterone, oestrone).

**PAPER: XI-P [Physical Chemistry Special]****CP: 4****Marks: 50****Unit–P-3111: Advanced Quantum Mechanics-I (2L/W; CP-2) Marks: 25**

**General Theory:** States of a physical state as vectors; orthonormality and closure property of eigen vectors; normalization by Dirac  $\delta$  function; coordinate and momentum representation of eigenstates;

**Variation Method:** Variation theorem; application to ground states of different systems; extension to excited states; linear variation; WKB Approximation; Matrix mechanics –Eigenvalues – Eigenvectors –Diagonalization.

**Perturbation Theory:**

**(i) Time independent formalism:** Rayleigh-Schrödinger theory for nondegenerate systems with simple applications; Brillouin Wigner Theory; Perturbation treatment in He atom; degenerate perturbation theory, Stark and Zeeman effects.

**(ii) Time dependent formalism:** Transition probability; Fermi Golden Rule; Einstein transition probabilities; spontaneous and induced emission. Rabi oscillation; Sudden Approximation, Gell-Mann and Low Theorem.

**Unit–P-3112: Electrode Dynamics (2L/W; CP-2) Marks: 25**

**Electrode Kinetics:** Simple Butler-Volmer (BV) eqn., symmetry factor, Tafel eqn. Exchange currents from low and high field approximation. D.L. effect on electrode kinetics. Generalised BV expression, Evaluation of kinetic parameters, transfer coeff. Stoichiometric no. and stoichiometric factor. Elucidation of some electrochemical reactions  $\text{Fe} \rightleftharpoons \text{Fe}^{2+} + 2\text{e}$ , hydrogen evolution (HE) reaction, Oxygen reduction reaction (ORR),  $\text{I}_2\text{-I}_3^-$  reaction etc. transient studies adsorption intermediates, Pseudocapacitance, roughness factor etc. Cyclic voltammetry and impedance studies Mechanism of charge transfer process across electrode-soln. interface, evaluation of  $i_0$  from theoretical consideration. Fundamentals of electroplating, corrosion, passivation, Batteries, fuel cells electrocatalysis and supercapacitors.

**Paper: XII-A [Analytical Chemistry Special] CP: 4 Marks: 50**

**Unit– A-3121: NMR, EPR, NQR and Mössbauer Spectroscopy**

**(2L/W; CP: 2) Marks: 25**

**NMR:** Identification of compounds like  $\text{H}_3\text{PO}_3$ ,  $\text{H}_3\text{PO}_2$ ,  $\text{HPF}_2$ ,  $\text{P}_4\text{S}_3$  etc. Factors affecting line width, evaluation of thermodynamic parameter with NMR, determination of reaction order, rate constant etc. from NMR. NMR spectra of paramagnetic ions. Effect of nature of bonds on spin-spin coupling. Contact shifts. Applications involving the magnitude of coupling constant –  $J_{13\text{C-H}}$ ,  $J_{\text{Pt-P}}$ ,  $J_{\text{P-F}}$  etc. NMR spectra of  $\text{B}_3\text{H}_8^-$ ,  $\text{HP}_2\text{O}_5^{3-}$ ,  $\text{TiF}_4 \cdot 2\text{B}$  (B as donor molecule); Integration and quantitative analysis. Double resonance technique. Pulse and FT NMR: Bloch equations, time domain vs. frequency domain, FID, CW vs. FT NMR, laboratory frame of reference, rotating frame of reference, relaxation time measurements, instrumentation.

**EPR:** Anisotropy of g-value, factors affecting the magnitude of g-value, Anisotropy in the hyperfine coupling constants, zero-field splitting and Kramers' degeneracy, Application.

**NQR:** Basic theory, quadrupole coupling constant, asymmetric parameters, effect of magnetic field in the spectra, relationship between 'q' and molecular structure, structural information from NQR spectra, Effect of quadrupole nuclei on EPR and NMR spectra. Application. Instrumentation.

**Mössbauer:** Gamma ray emission and absorption by nuclei, Mössbauer effect, Isomer shift, quadrupole splitting, magnetic interaction, use of Mössbauer spectra in chemical analysis. Instrumentation.

**Unit– A-3122:**

**CP: 2**

**Marks: 25**

**A-3122a : IR, Raman, CD and ORD Spectroscopy**

**(1L/W; CP: 1)**

**Marks: 12.5**

**Infrared Spectroscopy:** Origin, molecular vibrations in polyatomic molecules, potential energy of an oscillator, Harmonic Oscillator approximation, energy levels and selection rules, anharmonicity and its effect on energy levels and spectral features: overtones and hot bands, vibration-rotation spectra of diatomics: selection rules; P, Q and R branches; group vibration, limitation of the concept, FTIR, NDIR techniques.

**Raman Spectroscopy:** Theory, instrumentation and mechanism of Raman Effect in solids, liquids and gases. Classical and quantum mechanical treatment of rotational and vibrational Raman spectra of diatomics. Resonance Raman spectroscopy; Laser Raman spectra and application.

**CD and ORD spectrometry:** Experimental aspects, molecular dissymmetry and chiroptical properties, Cotton effect, Faraday effect in magnetic circular dichroism (MCD) and application.

**A-3122b: Atomic absorption and emission spectroscopy**

**(1L/W; CP: 1)**

**Marks: 12.5**

Basic theory, Flame atomization process, flames, nebulization, ionization, droplet prodipitation, mixing, desolvation, interference, lamps, burners, fuels. Nonflame atomization process, general discussion, high temperature furnaces, operating principles, process, interferences, advantages and disadvantages, hydride generation

analysis. Flow injection hydride generation. Quartz tube AAS (FI-Hg-QT-AAS). Applications.

Origin of spectra, technique, expectation sources, control and multisources, plasma discharge, instrumentation, qualitative analysis, advantages and disadvantages. Cp-AES, Application (general). Basic principle of inductively coupled plasma atomic emission spectrometry (ICPAES). Applications of AES and ICPAES

**Paper: XII-I [Inorganic Chemistry Special] CP: 4 Marks: 50**

**Unit– I-3121: Bioinorganic Chemistry (Advanced Level)**

**(2L/W; CP:2)**

**Marks: 25**

1. Transport of ions across membranes– Sodium-Potassium ion pump. Metal storage and transport proteins - transferrin , ferritin, ceruloplasmin and calmodulin . Electron transport proteins – cytochromes, ferredoxins and rubredoxins, blue copper protein. Redox metalloenzymes- Ascorbate oxidase, catalase, peroxidase, superoxide dismutase, cytochrome c oxidase.
2. Hydrolytic enzymes – carboxy peptidase, carbonic anhydrase.
3. Vitamin B<sub>12</sub> , Modelling of macromolecular metal complexes with special reference to coenzyme, hemoglobin. Photosynthesis: Chlorophyll, Photosystem I and II, Mn<sub>4</sub>O<sub>4</sub> cubane-complex. Interaction of metal ions with nucleic acids and their monomeric constituents- metal complexes of nucleosides and nucleotides, polynucleotides and native nucleic acids. DNA metal complex interaction.

**Unit-I-3122:**

**CP: 2**

**Marks: 25**

**I-3122a : Chemistry of smart materials**

**(1L/W; CP: 1) Marks: 12.5**

General definition of smart materials and smart systems, thermochromic, photochromic, piezochromic, electrochromic, piezoelectric, pyroelectric, thermo-/photo-actuating materials, shape memory material, polymorphic solids, self-healing materials, pH responsive materials, superhydrophobic materials.

**I-3122b : Advances in heterogeneous catalysis****(1L/W; CP: 1) Marks: 12.5**

Introduction, energy profile diagram, kinetics, Volcano plots, types of catalytic reactors, steps in a heterogeneous catalytic reaction, Factors affecting rate of reaction such as temperature, flow rates, molar composition, diffusion, particle size, shape etc. Concept of activity, selectivity, poisoning, promotion and deactivation. Thermodynamic consideration in surface reactions, mechanism of catalytic reactions, ammonia synthesis, methanol synthesis. Preparations and separations of the catalysts including zeolites, MCM-41, composite oxides and MOFs and use them in CO oxidation, selective oxidation, selective hydrogenation, organic reactions, biomass to liquid biofuels, CO<sub>2</sub> to fuels, etc. Photocatalytic and electrocatalytic water splitting and CO<sub>2</sub> reduction, green catalysis, environmental catalysis.

**Paper: XII-O [Organic Chemistry Special] CP: 4 Marks: 50****Unit– O-3121 : Organometallic Chemistry (2L/W; CP:2) Marks: 25**

Applications of Transition metals in Organic synthesis. Introduction, formalism and bonding. Organometallic reaction mechanism. Synthetic applications of complexes containing metal-carbon  $\sigma$ -bond: Heck, Kumada, Suzuki, Stille, Sonogashira and Negishi coupling reactions and their applications. Carbon monoxide insertion, Carbon-hetero-atom bond formation reactions. Palladium catalysed sequential reactions. Synthetic applications of metal alkenes and alkyne complexes: Applications of Pd(II)-salts. Cobalt-catalyzed reactions (Pauson-Khand and alkyne cyclotrimerization reactions). Applications of  $\eta^3$ -allyl palladium and nickel complexes. Applications of metal carbene complexes: Olefin Metathesis reaction and their applications (emphasized on RCM, CM, ROM and ene-yne metathesis). Chemistry of arene-chromium tricarbonyl complexes, reaction of Fischer and Schrock type carbene complexes, C-H activation,

**Unit– O-3122: Spectroscopy-II and Silicon Chemistry in Organic Synthesis****(2L/W; CP: 2)****Marks: 25**

NMR Spectroscopy of  $^{13}\text{C}$ ,  $^{15}\text{N}$ ,  $^{19}\text{F}$ ,  $^{31}\text{P}$  and  $^{17}\text{O}$  nuclei, DEPT, Difficulties and their remedies in scanning the spectra, relative utilities of different techniques available in scanning the spectra on routine basis. Frequency spreading for each of the nuclei, chemical shift scale, correlation of chemical shift. Scalar spin-spin as well as dipolar couplings and their applications. 2D and Multidimensional NMR spectroscopy: Utilisation of pulse for carrying out such processes. Relative advantages of such techniques with those of 1D spectroscopy. Homonuclear and heteronuclear correlation through bond, correlation through space and through exchange processes.

Advanced mass spectrometric techniques: Realization and application of different ionization techniques: Field ionization, SIMS, FAB, MALDI, ESI, Tandem mass spectrometry.

Comparison of typical properties of silicon and carbon. Application of silicon reagents in organic synthesis, e.g. protection of OH and NH groups by silylation, chemistry of acyl-, allyl-, aryl- and vinyl silanes; Peterson olefination reaction, sila-Pummerer rearrangement. Reactions of silylated diazomethane with aldehydes, ketones and aryl alkyl ketones. Dealkylation of esters, ethers and acetals by TMSCl/NaI, 1,2-carbonyl transposition etc.

**PAPER: XII-P [Physical Chemistry Special]****CP: 4****Marks: 50****Unit–P-3121: Advanced Statistical Mechanics-I****(2L/W; CP-2)****Marks: 25**

**Quantum Statistics:** Classical limits of Fermi-Dirac and Bose-Einstein distribution; Application of the quantum statistics for deriving thermodynamic properties of ideal BE and FD systems (conduction electron, black-body radiation, Bose Einstein condensation); density matrix.

**Imperfect gases:** Virial equation of state from grand partition function; second and third virial coefficients.

**Classical monatomic liquids:** Radial distribution function (RDF); Relating RDF with the thermodynamic properties; Integral equations; Potential of mean force; The direct correlation function

**Statistical mechanical perturbation theory of liquids:** Theory and its application to derive van der Waals equation of state.

**Unit– P-3122: Reaction Dynamics (2L/W; CP-2) Marks: 25**

**Kinetics of fast reactions:** Flow techniques, Kinetic equations of flow systems, Mechanism of Atom and Radical combination reactions, Flash photolysis and its application, Shock tubes and molecular beams. Dynamics of molecular motions, probing the transition state. Diffusion controlled and encountered reactions. Kinetics of enzyme catalyzed reactions, different types of mechanisms. Influence of pH, inhibitors and temperature on enzyme catalyzed reactions, Kinetics of surface reactions, Micellar Catalysis.

**Polymerization reactions:** condensation polymerization, free radical polymerization and ionic polymerization mechanisms, copolymerization reactions.

## Practical Papers

(8L [2days]/W; CP: 4)

**Paper: L-V-A [Analytical Chemistry Special Practical] CP: 4 Marks: 50**

Project oriented advanced synthesis/related studies

**Paper: L-V-I [Inorganic Chemistry Special Practical] CP: 4 Marks: 50**

Project oriented advanced synthesis/related studies

**Paper: L-V-O [Organic Chemistry Special Practical] CP: 4 Marks: 50**

1. Preparation of organic compounds and purification by chemical process, chromatographic process, resolution as applicable.

2. Estimation of drugs.
3. Estimation of tartaric acid and glucose by periodic acid method.

**Paper: L-V-P [Physical Chemistry Special Practical] CP: 4 Marks: 50**

1. (a) Determination of Standard Potential of  $\text{Ag}/\text{Ag}^+$  electrode and the solubility product of  $\text{AgX}$  from EMF measurements.  
(b) Determination of Standard potential of  $\text{Ag}-\text{AgX}$  electrode and calculation of activity coefficients of  $\text{HX}$ .  
(c) Determination of Ionisation constant of water,  $\text{HA}$  or  $\text{BH}^+$  type of acids using  $\text{H}_2$  and  $\text{Ag}-\text{AgX}$  electrodes.
2. Association constant in water by Fuoss and Kraus method (Computer analysis).
3. Determination of Counter ion binding of ionic micelles (CTAB) by  $\text{Ag}-\text{AgBr}$  electrode/ Conductometry.
4. (a) Determination of 'g' factor by ESR technique.  
(b) Determination of Band gap by the four probe method.
5. Determination of solvation number of  $\text{BaCl}_2$ / urea from the compressibility measurements by interferometer.
6. Phase studies of air water micro emulsion.
7. Chemical Actinometry: Intensity of Hg vapour lamp by uranylactinometer/ferrioxalateactinometer.
8. Formation Constant of charge transfer complexes by spectrophotometric method.
9. Oscillatory Reactions: Study by spectrophotometry/potentiometry.
10. Determination of Isoelectric pH of gelatin by viscometric measurements in the presence and absence of salt.

**Paper: L-VI-A [Analytical Chemistry Special Practical] CP: 4 Marks: 50**

Project related advanced analytical works

**Paper: L-VI-I [Inorganic Chemistry Special Practical] CP: 4 Marks: 50**

Project related advanced analytical works

**Paper: L-VI-O [Organic Chemistry Special Practical] CP: 4 Marks: 50**

1. Multi-step Organic Synthesis.
2. Extraction & purification of natural products (any two): Caffeine, Nicotine, Lycopene, Carotene etc.
3. Purity and molecular weight determination of a protein/ nucleic acid sample.

**Paper: L-VI-P [Physical Chemistry Special Practical] CP: 4 Marks: 50**

1. Determination of Activation parameters by studying the kinetics of alkaline hydrolysis of EtOAc.
2. Kinetic study of mutarotation of glucose and the determination of the catalytic coefficients by polarimetric method.
3. Study of the Salt, solvent and micellar effects on the rate of alkaline fading of crystal violet by spectrophotometric method.
4. (a) Reversible cyclic voltammetry of  $\text{Fe}(\text{CN})_6^{3-/4-}$   
 (b) Determination of  $I$  of H.E.R. of Pt surface from Tafel plot.  
 (c) Electrocapillary curves using dropping mercury electrode and evaluation of charge (gm) and surface excess quantities.
5. Verification of Ilkovic Equation, Heyrovsky Equation
6. Determination of unknown concentration of  $\text{Pb}^{2+}$  by  $\text{CrO}_4^{2-}$  and  $\text{SO}_4^{2-}$  by  $\text{Pb}^{2+}$  amperometrically.
7. Measurement and application of molar refraction.
8. Verification of Stern-Volmer equation by fluorescence quenching methods.
9. Synthesis and characterization of nanoparticles.
10. Determination of CMC mixed surfactants using tensiometer.
11. Potentiometric titration of halide mixtures.

## 4<sup>th</sup> Semester

### Theoretical Papers

**PAPER: XIII-A [Analytical Chemistry Special] CP: 4 Marks: 50**

**Unit-A-4131: CP: 2 Marks: 25**

**A-4131a : Statistical and computational methods in Analytical Chemistry**

**(1L/W; CP:1) Marks: 12.5**

Introduction to error analysis: systematic error, random error, standard deviation, standard error of mean, Coefficient of variation, standard deviation of calculated results, Significant figures, Confidence interval and confidence limit. Hypothesis testing, null hypothesis, comparison between experimental mean and known value- z test, t test, Detection of gross error- Q test, methods of least squares.

**A-4131b : Advanced Electroanalytical Techniques**

**(1L/W; CP:1) Marks: 12.5**

High Frequency Titrations- Basic concept, application. Ion selective Electrodes- Principles and applications.

Electrogravimetry: Constant current electrolysis and controlled potential electrolysis – principles and applications. Primary and Secondary Coulometry

Linear Sweep Voltammetry (LSV) and Cyclic Voltammetry (CV). Ellipsometry, Internal Reflection Spectroelectrochemistry (IRS), Infrared Spectroelectrochemistry (IR-SEC).

A.C. Polarography with tensametry, Applications.

**Unit-A-4132: CP: 2 Marks: 25**

**A-4132a : Advanced Level Treatment of Solvent Extraction**

**(1L/W) Marks: 12.5**

Liquid-liquid extraction: Batch extraction, continuous extraction and continuous counter-current extractions- principles, apparatus, methods and their applications and uses in chemical separations.

Synergic extraction, ion-pair or ion association extraction, extraction by equilibrium shifts.

Solid-liquid extraction: principles, apparatus, methods; discontinuous infusion type extraction, application to the separation of alkali and alkaline earth metals. Application of solid-liquid extraction in: extraction of herbal product, pharmaceutical and paint industry.

**A-4132b : Advanced Level Treatment of Chromatography**

**(1L/W; CP:1)**

**Marks: 12.5**

Chromatography: classification, principle and efficiency of the technique. Mechanism of separation: adsorption, partition & ion exchange. Development of chromatograms: frontal, elution and displacement methods. Qualitative and quantitative aspects of chromatographic methods of analysis: IC, GLC, GPC, TLC and HPLC.

Stereoisomeric separation and analysis: Measurement of optical rotation, calculation of enantiomeric excess (ee)/ diastereomeric excess (de) ratios and determination of enantiomeric composition using NMR, Chiral solvents and chiral shift reagents. Chiral chromatographic techniques using chiral columns (GC and HPLC).

Gas chromatography, liquid chromatography, supercritical fluids, Importance of column technology (packing, capillaries), Separation based on increasing number of factors (volatility, solubility, interactions with stationary phase, size, electrical field), Detection: simple vs. specific (gas and liquid), Detection as a means of further analysis (use of tags and coupling to IR and MS), Electrophoresis (plates and capillary) and use with DNA analysis.

**PAPER: XIII-I [Inorganic Chemistry Special]**

**CP: 4**

**Marks: 50**

**Unit-I-4131: Applications of Group Theory in Chemistry:**

**(2L/W; CP: 2)**

**Marks: 25**

1. Systematic Reduction of reducible representations including the representation with imaginary character. Direct Product of Irreducible representations.
2. C-F splitting of orbital degeneracy of free ions under  $D_{4h}$ ,  $T_d$  and  $O_h$  symmetries.
3. Bethe's method of descending symmetry. Strong field – weak field correlation diagram for  $d^2$  &  $d^3$  systems ( $O_h$  and  $T_d$  symmetry)

4. Double Groups and constructions of Character table for  $D_4'$  and  $O'$ . Effect of spin-orbit coupling on C-F states in  $D_{4h}$  and  $O_h$
5. Theoretical considerations – normal modes and normal coordinates of vibration; Symmetry of normal vibration, normal mode analysis, selection rules for IR and Raman transitions for linear and non linear molecules ( $C_{2v}$ ,  $C_{3v}$ ,  $C_{4v}$ ,  $D_{2h}$ ,  $D_{3h}$ ,  $D_{4h}$ ,  $T_d$  and  $O_h$  symmetries).
6. Group theoretical considerations of vibronic coupling. Consequences of vibronic coupling on the spectroscopic properties of transition metal complexes.
7. Tanabe-Sugano diagrams – principles of construction; estimation of interelectronic repulsion/CF parameter; interpretation of electronic (absorption) spectra of transition metal complexes.
8. Physical origin of Jahn-Teller effect; Derivation of Jahn-Teller theorem from group theoretical principles; Structural consequences of Jahn-Teller effect in transition metal complexes; examples for tetrahedral, octahedral etc geometries

**Unit– I-4132: Insight into Chemical Bonding (2L/W; CP: 2) Marks: 25**

1. Empirical MO – Hückel theory; examples.
2. Symmetry adapted MO – Symmetry and group theoretical methods for qualitative MO energy level diagrams of  $AH_n$  and  $AB_n$  ( $n = 1$  to  $6$ ) types of molecule. Analogous MO treatment for the transition metal complexes.
3. MO energetics model (Walsh's diagram). Study of the variation of energy of MOs with the change of bond angle. Construction of Walsh correlation diagram for  $AB_n$  ( $n = 2$  to  $4$ ) types of molecule.

***Shapes of smaller molecules – theoretical modes:***

- (i) Concept of Valence Bond – VSEPR model – Hybrid AO sets of geometry of the molecules, theoretical idea about the bond angles; qualitative assessment of the effects of mutual repulsion of the bonded and non-bonded electron pairs on angular distortions; examples.
- (ii) Symmetry and group theoretical methods for construction of Hybrid orbitals.

**Relativistic Effects and its consequences in inorganic and organometallic chemistry:**

Theoretical considerations of relativistic effects, direct and indirect relativistic effects, comparison of direct and indirect relativistic effects for elucidating the properties of heavier elements; Consequences of relativistic effects toward transition and post transition sixth row elements with special reference to (a) variation of IE and EA along the group (b) stabilization of high oxidation state in third transition elements (c) coloration of coinage metals, (d) aurophilicity, (e) formation of auride ion, (f) liquid nature of mercury, (g) inert-pair effect, (h) hyper coordination of second period elements etc.

**PAPER: XIII-O [Organic Chemistry Special] CP: 4 Marks: 50**

**Unit– O-4131 : Radical Chemistry, Polyene Cyclization and Diazoketone**

**Chemistry (2L/W; CP:2) Marks: 25**

Basic principles, Functional group transformations via Barton Esters, C-C bond formations by various radical-radical and radical-non-radical coupling reactions. Chain reaction based on stannane chemistry. Syntheses of natural products by using radical reaction as the key steps. Organo samarium and organo titanium reagents. Reduction with iron, copper, ruthenium salts. Dissolving metal reductions. Various ring expansion, ring contraction, remote functionalization and radical fragmentation reaction.

Polyene cyclisation: Synthesis of polycyclic systems using acetals as initiator and double bond as terminator. Chemistry of  $\alpha$ -methylene- $\gamma$ -butyrolactone system.

Diazoketone chemistry: Synthesis of various bridged polycyclic systems by acid catalysed decomposition of various  $\alpha$ -diazoketone derivatives. Chemistry of  $\beta,\gamma$ -unsaturated  $\alpha$ -diazoketone.

**Unit– O-4132 : Linear Free Energy Relationship and Supramolecular Chemistry****(2L/W; CP: 2)      Marks: 25**

Hammett equation and its modifications, Separation of Inductive and resonance effects- $\sigma_I$  and  $\sigma_R$  scales, Taft equation, Yukawa-Tsuno equation, Elucidation of reaction mechanisms, Application of Hammett correlation to heterocyclic systems, Thermodynamic aspects of Hammett equation, Dual substituent parameter (DSP) and Dual substituent parameter-non-linear resonance (DSP-NLR) correlations-Taft-Bromilow-Brownlee approach.

From molecular to supramolecular chemistry: non-covalent interaction. Synthetic molecular receptors for anion, cation and neutral molecules; Preorganization and their functions, Hamilton receptor, Aromatic electron donor-acceptor conformer, Supramolecular reactivity and catalysis, Supramolecular sensors, catenanes, rotaxanes, molecular Knots, Borromean ring, Supramolecular machines, switching devices, molecular shuttle, molecular motor, molecular valve, rotary motor, supramolecular aggregates and Nanotechnology, Artificial Receptors for Biomolecules, Molecular recognition at the membrane-water interface and inside the membrane, Membrane fusion through molecular recognition.

**PAPER: XIII-P [Physical Chemistry Special]      CP: 4      Marks: 50****Unit– P-4131: Advanced Quantum Mechanics II (2L/W; CP:2)      Marks: 25**

**Many-electron-atoms:** Many electron wave function including spin eigen functions of  $S^2$ ,  $S_z$ ,  $L^2$ ,  $L_z$  operators, Quantum mechanical treatment of spin-orbit interaction; elementary treatment of Hartree-Fock SCF, Post HF treatment (CI, DFT, MCSCF etc.).

**Molecular Systems:** Homonuclear and heteronuclear diatomic molecules; vibrational and rotational wavefunctions; Morse oscillator wavefunction.

Hückel theory for linear and cyclic conjugated systems; electron density and bond order; extended Hückel theory; semiempirical methods.

**Forces in molecules:** Virial theorem, Hellman-Feynman theorem applications.

**Unit– P-4132: Interfacial Electrochemistry** (2L/W, CP:2) **Marks: 25**

**Double layer (DL) across electrified interface:** Genesis of DL, potential difference across interface; polarizable and non polarizable interface, electrocapillary thermodynamics, surface excess quantities from electrocapillary and capacitance measurements structure of the DL,: HB, GC. Stern and BDM models, capacitance hump and contact adsorption; specific adsorption and Esin Markov coefficient. Electrosorption of solvent dipoles, neutral organic solutes from flip-flop model. Langmuir, Frumkin and Temkin electro-adsorption.

**Structure of semiconductor solution interface:** distribution of GB space charges, potential and capacitance, flat band potential, Mott-schottky equation. Basic concept and equations relating eletromechemical kinetics across SC-soln. Interface. Behaviour of extrinsic SC-soln interface, PEC Photoelectrochemical solar cells, photo-electrochemistry.

**PAPER: XIV-A [Analytical Chemistry Special]** **CP:4** **Marks: 50**

**Unit-4141:** **CP:2** **Marks: 25**

**A-4141a: Application of spectrophotometry & spectrofluorimetry in bioanalytical chemistry** **(1L/W; CP:1)** **Marks: 12.5**

Application of spectrophotometry in the quantitative estimation of biological macromolecules like DNA and Proteins. Application of spectrofluorimetry in detection and estimation of representative biomolecules (both fluorescent and non-fluorescent). Assay of very low quantity of vitamin B<sub>1</sub> in food stuffs; NADH, hormones (triiodothyronine, thyroxine & insulin), drugs (amoxicillin and alprazolam), pesticides (DDT & malathion), cholesterol, porphyrin in biological samples and preparation of the sample for performing the above experiments.

**A-4141b: Ultracentrifugation & gel electrophoresis (Basic principle and applications)** **(1L/W; CP:1)** **Marks: 12.5**

Ultracentrifugation: principles of sedimentation, preparative ultracentrifugation and analytical ultracentrifugation. Application of Ultracentrifugation in separating bio-molecules and determining their mass.

Gel electrophoresis: principles, nature of various types of gels, their applications in separating bio-molecules and determining their mass. 2D gel electrophoresis and its applications.

**Unit-A-4142:**

**CP:2**

**Marks: 25**

**A-4142a : Environmental Chemistry (1L/W; CP:1)      **Marks: 12.5****

1. Environmental segments: atmosphere, hydrosphere, lithosphere, and biosphere. Environmental cycles: water, oxygen, nitrogen, carbon, phosphorus, and sulfur cycles, composition and structure of the atmosphere, chemical and photochemical reactions in the atmosphere, ozone layer and its importance, Major air pollutants and their sources, greenhouse effect, acid rain, photochemical smog, air pollution control measures.

2. Pollution caused by SO<sub>2</sub>, CO<sub>2</sub>, CO, NO<sub>x</sub>, H<sub>2</sub>S and other foul smelling gases, Carbon monoxide emissions, effects, uses, poisoning symptoms, Methods of estimation of CO, NO<sub>x</sub>, SO<sub>x</sub> and control procedures, Control of particulate matter: PM 10 and PM 2.5 and their harmful effects, Real-time Air Quality Index (AQI).

3. Environmental role of water, major water pollutants: Physical, Chemical, Biological and Physiological, water quality parameters, water treatment: domestic, industrial, waste water treatment, chemical treatment and microbial treatment, water quality standards: DO, BOD, COD, TDS and hardness parameters, Electrodialysis desalination for water and waste water.

**A-4142b : Analytical Techniques for Food and Drug Analysis:**

**(1L/W; CP:1)**

**Marks: 12.5**

1. Different methods of analysis of carbohydrate, protein and fat/lipids.
2. Methods of analysis of Food preservatives: Selected examples
3. Milk: Composition of milk, analysis of pH, acidity, fates, casein content, lactose content, mineral content in the commercial milk. Adulteration of milk.
4. Active Pharmaceutical Ingredients (API), Different types of drugs (antiviral, analgesic, anti-inflammatory, antipyretic, antimalarial, sedative etc), Role of Food and Drug Administration (FDA) and FSSI (in India). Stability studies and self life determination.

5. Tabletability test for drugs like Tablets and Capsules, dissolution test of tablets and capsules, analysis of moisture / water content (Karl-Fischer titration).

**PAPER: XIV-I [Inorganic Chemistry Special] CP: 4 Marks: 50**

**Unit– I-4141 : Magnetochemistry (2L/W; CP: 2) Marks: 25**

1. Magnetic Substances: Terminology related with magnetic properties, Classification, Cooperative Magnetism, Ferromagnetic substances and related aspects, Application of hard and soft ferromagnetic substances.
2. Para-, ferro- and antiferro-magnetism: Temperature dependence of magnetic susceptibility, Curie's Law and Curie-Weiss Law, Pathways of ferro- and antiferro-magnetism, magnetic properties of an electron, paramagnetism and thermal energy, Spin-orbit Coupling, Lande Interval Rule, Mixing of the ground state with the excited states, Spin Crossover, Temperature Independent Paramagnetism (TIP).
3. Diamagnetism: Origin, Lorenz's law, Pascal's constants and diamagnetic susceptibility.
4. Magnetic properties of compounds of d and f block elements: concentrated and dilute systems.
5. Other important magnetic systems and phenomenon: Ferrimagnetism, meta-magnetism, Spin Canting, Magnetically frustrated systems, single molecule magnet (SMM), single ion magnet (SIM), single chain magnet (SCM).

**Unit-I-4142: CP: 2 Marks: 25**

**I-4142a : Inorganic Reaction Mechanism II (1L/W; CP: 1) Marks: 12.5**

General characteristics and classification of redox reactions. Mechanism of electron transfer reaction. Self-exchange reaction. Frank-Condon Principle (non-mathematical treatment). Outer sphere and inner sphere reactions. Applications of Marcus expression (simple form). Redox catalyzed substitution reactions. Catalyzed redox reactions, substitution controlled redox reactions.

**I-4142b: Metals in medicines****(1L/W; CP:1)****Marks: 12.5**

1. Metallo-Drugs and Their Action, Platinum Drugs for Treating Cancer: Cisplatin, Carboplatin, Oxaliplatin
2. Anticancer Agents Beyond Cisplatin: Ruthenium and Gold Anticancer Agents, Titanium and Gallium for Treating Cancer and Other Anticancer Active Metal Complexes
3. Metal Complexes for Treating Arthritis and Diabetes: Chemistry of Gold in Biological Media, Gold Compounds for Treating Arthritis, Vanadium Compounds for Treating Diabetes
4. Metal Complexes for Killing Parasites, Bacteria and Viruses: Malaria, Tuberculosis, Peptic Ulcer Disease, Syphilis, Bacterial Infections, Acquired Immunodeficiency Syndrome (AIDS)
5. Metal Ion Imbalance in the Body: Alzheimer's Disease, Wilson's Disease, Menkes Disease, Beta-Thalassemia, Iron-Deficiency Anemia, Calcium Imbalance, Chelation Therapy
6. Metal Complexes for Detecting Disease: Technetium in Diagnostic Nuclear Medicine, Metal Compounds as Contrast Agents for MRI

**PAPER: XIV-O [Organic Chemistry Special]****CP: 4****Marks: 50****Unit– O-4141 : Asymmetric Synthesis****(2L/W; CP: 2)****Marks: 25**

Syntheses of chiral compounds applying Chiron approach, ideas of diastereoselective and enantioselective reactions, basic principles and salient features of asymmetric synthesis, chiral auxiliaries (applications, merits and demerits), asymmetric epoxidation, dihydroxylation and aminohydroxylation, asymmetric oxidations of sulfides to sulfoxides, syntheses of commercially and pharmaceutically important chiral compounds using chiral catalysts mainly developed by Knowles, Noyori and Sharpless, asymmetric synthesis of Crixivan (anti-aids compound), asymmetric reduction of unsymmetrical ketones with BINAL-H and CBS reagents, application of

chiral oxazaborolidine in the asymmetric Diels-Alder reaction (specially, for the synthesis of the common precursor of prostaglandins), asymmetric transformations using chiral phase transfer catalyst, asymmetric C-C bond formation using chiral N-heterocyclic carbene, asymmetric epoxidation of unfunctionalized olefins, principle and applications of asymmetric organocatalysis, applications of bio-catalysis.

**Unit– O-4142 : Total Synthesis of Natural Products (2L/W; CP: 2) Marks: 25**

Synthesis of some important terpenoids (Longifolene, dehydroabietic acid and abietic acid,  $\beta$ - amyryn, taxol), alkaloids (reserpine, morphine, quinine, strychnine) with emphasis on retrosynthetic analysis.

**PAPER: XIV-P [Physical Chemistry Special] CP: 4 Marks: 50**

**Unit– P-4141: Non-Equilibrium Thermodynamics (2L/W; CP:2) Marks: 25**

Entropy production in irreversible rate processes. Different types of forces and fluxes, coupling of irreversible rate processes; Curie Prigogine symmetry principle. Phenomenological eqns in linear region. Onsager Reciprocity Relation: Theory of fluctuation, Microscopic reversibility & linear regression. Stationary state and equilibrium States; their differences. Principle of minimum entropy production. Application of linear region of non-equilibrium thermodynamics: Thermoelectric effect (Seebeckemf, Peltier heat & thermoelectric power); Thermomechanical effect (Soret, Dufour, Knudsen & Mechanocaloric effects); Electrokinetic effect (Electro osmosis, electro osmotic pressure, streaming current and streaming potential). Phenomenological eqn. in non-linear region, Prigogine Glansdorf theorem, Oscillation about stationary state, Bistability, Oscillatory reactions.

**Unit– P-4142: Photochemistry and Spectroscopy (2L/W; CP:2) Marks: 25**

1. Interaction of electromagnetic radiation with molecule: Einstein's treatment on two level transitions, Transition moment integral and its relation with molar extinction coefficient. Basis of selection rule from symmetry argument, Franck Condon principle and its violation, Oscillator strength, Nature of transitions (e.g.,  $n-\pi^*$ ,  $\pi-\pi^*$ ,  $d-d$ ,

charge transfer etc.), vibronic and spin-orbit coupling, solvent effect on absorption spectra.

2. Jablonski diagram, Fluorescence and phosphorescence, Kasha's Rule, Solvent effect on emission spectra, Stoke's shift, Quantum yield, Delayed fluorescence, Fluorescence quenching (dynamic and static), Stern - Volmer equation, Energy transfer (Forster's dipole coupling), Electron Transfer phenomenon (Marcus theory, Rehm Weller theory), Proton transfer phenomenon, complex formation (excimer, exciplex).

3. Properties of electronically excited molecules: Redox potential, dipole moment,  $pK$  values, Fluorescence life-time, Potential energy diagram for donor acceptor system, Fluorescence anisotropy and its use.

4. Nonradiative intramolecular electronic transition, internal conversion, inter-system crossing, Crossing of potential energy surface (Franck-Condon factor), Adiabatic and non-adiabatic cross over, Photoacoustic spectroscopy: Principle, technique and applications.

5. Mössbauer spectroscopy: Principles, technique, chemical shift, quadruple effect, effects of magnetic field, applications.

6. Photoelectron spectroscopy & X-ray fluorescence spectroscopy: Basics and applications.

**PAPER: XV-A [Analytical Chemistry Special] CP: 4 Marks: 50**

**Unit- A-4151 : Molecular Fluorescence and Phosphorescence Spectroscopy, Chemiluminescence and XRF (2L/W; CP: 2) Marks: 25**

Basic theory, instruments, different photonic and deactivation process (interval conversion, vibration, relaxation, intersystem crossing fluorescence, phosphorescence, external conversion etc.), energy level diagram, Morse curve; fluorimetric reagents, effect of substitution (on aromatics) upon photoluminescence, structural and environmental effects on photoluminescence, quenching and non-quenching extinction of fluorescence and probable mechanism for quenching,

characteristics of  $\pi$ - $\pi$  states, spectra, mirror image file, its violation and causes of violation delayed fluorescence, charge transfer process, fluorescence, immunoassay and its advantages, cations and anion sensing fluorescent molecules. Fields of applications, assessment as an ultratrace analysis technique. Principal types of reactions used in fluorimetric analysis. Different Applications. Low temperature phosphorescence, Room temperature phosphorescence (RTP).

**Chemiluminescence:** Theory, measurement of chemiluminescence, mechanisms in analytical applications.

**XRF:** Basic principle, instruments, excitation sources, energy dispersive and wavelength dispersive XRF techniques – their advantages and disadvantages, matrix effects and their suppression, health hazards and safety applications.

**Unit-A-4152**

**CP:2**

**Marks: 25**

**A-4152a : Radiochemical Methods of Analysis (1L/W) Marks: 12.5**

**Radio-chemical technique:** working principles in radiochemical laboratory. Role of carrier, isotopic exchange reaction and applications. Principles, applications and problems of neutron activation analysis. Radio-active reagents in the analysis of trace element.

**Radio Analytical Chemistry:** Interaction of radiation with matter. Principles of construction of a Geiger Muller Counter, proportional counter, scintillation counter, Scaler's counter, pulse–height analyzer, photomultiplier tubes. Low level counting devices. Radiation chemistry: introduction, interaction of radiation with nucleic acid in aqueous solution. Radiation dosimetry- Physical dosimetry, Chemical dosimetry (Ferrous sulphate and Cerric sulphate dosimetry), Glass dosimetry

**A-4152b :Thermal method of analysis: Instrumental approach**

**(1L/W)**

**Marks: 12.5**

Brief Introduction to different types of thermal analysis: Thermogravimetric analysis (TGA), Differential thermogravimetric analysis (DTG), Differential thermal analysis (DTA).

Differential Scanning Calorimetry (DSC): a brief outline and a comparative discussion of DSC with DTA.

Instrumentation TG, DTA and DSC- Basic principles, evolution of the instruments. Systematic flow diagram, methodology of design and electronic devices related to the instrument. Computer interface and troubleshooting of the equipment. Hyphenation of the instrument and evolve gas analysis.

Factors affecting the results of thermal analysis.

Applications of different thermal methods of analysis. Understanding of desolvation/deaquation, phase transition. Automatic thermogravimetric analysis – single, binary, ternary systems. Quantitative DTA, peak area and its equations.

Different types of thermometric titrations and their applications.

**PAPER: XV-I [Inorganic Chemistry Special] CP: 4 Marks: 50**

**Unit-I-4151: CP:2 Marks: 25**

**I-4151a : NMR Spectroscopy (1L/W; CP:1) Marks: 12.5**

**NMR:** Identification of compounds like  $\text{H}_3\text{PO}_3$ ,  $\text{H}_3\text{PO}_2$ ,  $\text{HPF}_2$ ,  $\text{P}_4\text{S}_3$  etc. Factors affecting line width, evaluation of thermodynamic parameter with NMR, determination of reaction order, rate constant etc. from NMR. NMR spectra of paramagnetic ions. Effect of nature of bonds on spin-spin coupling. Contact shifts. Applications involving the magnitude of coupling constant-  $J_{13\text{C-H}}$ ,  $J_{\text{Pt-P}}$ ,  $J_{\text{P-F}}$  etc. NMR spectra of  $\text{B}_3\text{H}_8^-$ ,  $\text{HP}_2\text{O}_5^{3-}$ ,  $\text{TiF}_4 \cdot 2\text{B}$  (B as donor molecule); Simplification of complex spectra: shift reagents, double resonance, NOE, spin tickling. Pulse and FT NMR: Bloch equations, time domain vs. frequency domain, FID, CW vs. FT NMR, laboratory frame of reference, rotating frame of reference, relaxation time measurements.

**I-4151b : EPR, NQR and Mössbauer Techniques (1L/W; CP:1) Marks: 12.5**

**EPR:** Anisotropy of g-value, factors affecting the magnitude of g-value, Anisotropy in the hyperfine coupling constants, zero-field splitting and Kramers' degeneracy, Application.

**NQR:** Basic theory, effect of magnetic field in the spectra, relationship between 'q' and molecular structure. Structural information from NQR spectra, Applications.

**Mössbauer:** Gamma ray emission and absorption by nuclei, Mössbauer effect, examples. Isomer shift, quadrupole splitting, magnetic interaction, information of spin and oxidation states, structure and bonding, spin transition from spectra of different Mossbauer active nuclei in variety of environments Use of Mössbauer spectra in chemical analysis.

### **Unit-I-4152: MOLECULAR AND SUPRAMOLECULAR PHOTOCHEMISTRY**

**(2L/W, CP:2)**

**Marks: 25**

1. **Introduction:** What is photochemistry; Excited states as new chemical species: different energy, lifetime, geometry, dipole moment, redox and acid/base properties, and reactivity. Deactivation processes of electronic excited states: rate constants, efficiencies, quantum yields. Lifetimes of an electronic excited state: definition and relation to deactivation rate constants.

2. **Radiative and radiationless processes:** molecular wave functions and Born-Oppenheimer approximation. Probability and selection rules for radiative transition of absorption, spontaneous and stimulated emission, and for radiationless transitions. Frank-Condon principle, Jablonski diagram: approximation and information that can be obtained from it. Correlation between absorption/emission spectra and the corresponding Jablonski diagram. Potential energy curves and surfaces for ground and electronic excited states of simple molecules.

3. **Bimolecular quenching processes** involving electronically excited states: Stern-Volmer equation, excimers and exciplexes. Catalyzed deactivation, photoinduced energy- and electron-transfer. Examples of quenching experiments by measurements of excited state lifetimes and emission quantum yields: static and dynamic quenching.

3.1 **Electronic energy transfer:** Coulombic and exchange mechanisms; spin selection rules and distance dependence. Applications of sensitization and quenching processes.

3.2 **Photoinduced electron transfer:** redox potential of electronic excited states. Examples of photocatalysis, conversion of light into chemical energy and vice versa (chemiluminescence and electrochemiluminescence).

4. **Laser:** Principles of lasers. Examples of the most commonly used lasers. Applications in photochemistry. Basic concepts of time-resolved measurements for identifying transient species (laser-flash photolysis)

5. **Brief account on supramolecular photochemistry and analysis of some complex systems** (such as Dendrimers and Molecular Machines): from design to application. Molecular wires and switches for photoinduced electron and energy transfer: systems based on metal complexes. Light-harvesting antennae. Molecular recognition of cations, anions and molecules with different receptors. Overview, from history to state of the art, on the applications of the photochemistry in nanotechnology (LED and OLED, solar energy conversion, photocatalysis, bio-applications, new materials).

**PAPER: XV-O [Organic Chemistry Special] CP: 4 Marks: 50**

**Unit– O-4151 : Carbohydrate Chemistry (2L/W; CP:2) Marks: 25**

Synthesis of deoxy- and aminodeoxy sugars; Synthesis of oligosaccharides (Protection and deprotection of carbohydrate systems, Glycosidation techniques) and oligosaccharide synthesis (including one example of combinatorial oligosaccharide/polysaccharide synthesis); Carbohydrate-Chiral pool synthesis (simple molecules).

**Unit– O-4152 : Medicinal Chemistry (2L/W; CP:2) Marks: 25**

1. Pharmacodynamics and pharmacokinetics and Drug design and synthesis of drugs, synthesis and chemistry of vitamins.
2. **Vitamins:** Definition of vitamins and coenzymes, classification of vitamins, mechanism of function with synthesis of vitamin A, D, E, B1, B2, B5, B6, C, H (Biotin) and Folic acid etc.

3. **Drugs:** Introduction, Classification of drugs, brief discussion of drug targets, Drugs based on enzyme inhibition: Sulfa drugs, penicillin antibiotics and fluorouracil (Mechanism of drug action). Drug targets on nucleic acids (Alkylating agents and intercalating agents). Definition of antagonist, agonist, prodrugs, pharmacokinetics and pharmacodynamics, concept of structure-activity relationship (SAR) and quantitative structure-activity relationship (QSAR).

**PAPER: XV-P [Physical Chemistry Special] CP: 4 Marks: 50**

**Unit– P-4151: Advanced Statistical Mechanics-II (2L/W; CP:2) Marks: 25**

**Non-equilibrium Statistical Mechanics:** Random processes; Time-correlation functions; Brownian motion; Langevin equation for random motion; Time dependence of fluctuation; Fluctuation-dissipation theorem; Fokker- Planck equation.

**Introduction to Simulation Methods :** The Idea of Molecular Dynamics Simulation; Concepts of Initialization, The Force Calculation, Algorithm for Integrating Equations of Motion; An Application (Monatomic liquids); Introduction to The Monte Carlo Method; A basic Monte Carlo Algorithm.

**Unit– P-4152: Biophysical Chemistry (2L/W; CP:2) Marks: 25**

Hydrophobic effect and self organizing systems, Structure and functions of proteins and nucleic acids and their stability. Structure and functions of cell membranes. Ion transport through cell membrane and nerve conduction. Multiple equilibria; stacking and co-operative interactions in biological systems. Muscle contraction.

Techniques for study of structure & function of proteins and nucleic acids. Structure and function of cell membranes. Ion transport through cell membrane and nerve condition. Multiple equilibria, staking and cooperative interactions in biological systems. Muscle contraction.

**PAPER: XVI-A [Analytical Chemistry Special] CP: 4 Marks: 50**

**Unit-A-4161: CP: 2 Marks: 25**

**A-4161a: Advanced Microscopic Techniques: (1L/W; CP:1) Marks: 12.5**

1. Electron-materials interactions, Sources: Tungsten filament, Solid state crystal (Cerium hexaboride or Lanthanum hexaboride), Field emission gun (FEG), FESEM, EBSD-Camera resolution, HRTEM, HAADF, STEM, Role of an elastic and non-elastic electrons for digitization of images, Bright and Dark field images, Electron energy loss spectroscopy (EELS), Continuum X-ray analysis are essential parts for the analysis of different crystallite nature, atomic planes and compositional/purity of samples/phases.
2. AFM/EFM analysis for different samples: Grain size, degree of deformation, phase type and particle size distribution (PSD), calculation of different roughness parameters and its utility in different sensor quality.
3. 3D Surface Profilometer- Non-Contact Profilometers for thickness/roughness parameters from the surface topography of deposited materials/sensors.

**A-4161b : Nanomaterials (1L/W; CP:1) Marks: 12.5**

1. Different synthetic routes: Physical, Chemical, Mechanical and electrochemical methods of nanomaterial design, Control of growth kinetics/seeding kinetics, morphology and structure, Classifications of nanosystems: 0D, 1D, 2D, 3D Nanomaterials, Size dependent properties of nanomaterials - Quantum Confinement Effects, Electronic properties and their optical behavior changes, Surface Plasmon Resonance (SPR), Direct and Indirect Transitions: Optical phenomena in nanoscale Materials
2. Hybrid organic-inorganic nanomaterials (functionalized nanomaterials) and its wide application towards different sensor, SAMS (self-assembly of monolayers) films, Core-shell nanosystems, Bimetallic sensor probes, Janus particle, Different types of nanoclusters, Metcars and other energy harvesting materials and their applications in different areas.

3. Nanolithographic techniques, Microelectromechanical systems: fabrication, design and Applications: MEMS and NEMS devices, Electrochemical sensors and biosensors.

4. Application to Environment: waste reduction and water treatment strategies. Nanotoxicology: toxicological properties of nanoparticles (NPs).

**Unit– A-4162 : Kinetic Methods of Analysis (2L/W; CP:2) Marks: 25**

Introduction: Concept of terms like degree of advancement of a chemical reaction, stoichiometry, rate laws, mechanism, etc. Derivation of some complex rate laws and their interpretation. Comparison of kinetic and non-kinetic methods of analysis: Where and why kinetic methods of analysis becomes the last resort of conventional analyses? Measurements of reaction rates – slow and fast reactions.

Catalysed reactions: Kinetic methods for homogeneous catalysed solution reactions and determination of catalysts. Complementary and non-complementary redox reactions; Kinetic methods for uncatalysed reactions. Kinetic methods for in-situ determination of closely related mixtures. Enzyme catalysis: Theory and application, determination of enzymes, substrates, activators and inhibitors

Examples chosen from real life; viz. estimation of iodide in common salt, mercury in environment, fluoride in water or toothpaste, double bonds in polymers, alcohol in blood, enzymes like lactate dehydrogenase, isocitrate dehydrogenase, etc. Error analysis in kinetic determination.

**PAPER: XVI-I [Inorganic Chemistry Special] CP: 4 Marks: 50**

**Unit– I-4161: Organometallic Chemistry and Catalysis (2L/W;CP:2) Marks: 25**

1. Brief discussion on types of metal-carbon bonded complexes; selected examples of M-C  $\sigma$ - and  $\pi$ -bonded complexes; general strategies for their synthesis.
2. Reactions Involving CO ligand, Insertions Involving Alkenes, Other Insertions,  $\alpha$ ,  $\beta$ ,  $\gamma$  and  $\delta$  Elimination, De insertion and Nucleophilic and electrophilic attack on CO-ordinated ligand, instability (decomposition pathway) and stabilization.

3. Basic aspects of molecular catalysis: Pre-catalyst (or catalyst-precursor), catalyst loading, optimization of experimental parameters, catalytic cycle, conversion and yield; Catalytic efficiency: turnover number (TON) and turnover frequency (TOF).
4. Organometallic chemistry and catalysis (with emphasis on nature of catalyst, mechanism of catalysis and involvement of organometallic species in the catalytic cycle): C-C and C-N coupling reactions; hydrogenation (including transfer-hydrogenation) of olefins; hydroformylation reaction; hydroamination reaction.
5. Transition metal carbene complexes: Fischer carbenes and Schrock carbenes; N-heterocyclic carbenes (NHCs); synthesis, structure and reactivity; Grubbs catalyst (1<sup>st</sup> generation and 2<sup>nd</sup> generation): Synthesis, structure, applications in olefin metathesis, mechanism.
6. Utilization of arene complexes in catalysis; potential of arene complexes in medicinal chemistry.

**Unit-I-4162****CP: 2****Marks: 25****I-4162a :Electrochemistry****(1L/W; CP:1)****Marks: 12.5**

***Cyclic voltammetry, DPV and coulometry:*** Linear Sweep Voltammetry (LSV) and Cyclic Voltammetry (CV), CV: a logical extension of LSV, Basic principles, three electrode system, Randles-Sëvcik equation, reversible, quasi-reversible, irreversible cyclic voltammograms; Differential Pulse Voltammetry (DPV); electrosynthesis, electrocatalysis, electropolymerisation, spectroelectrochemistry, Surface modifications, EC, ECE etc. pathways, protic-electroprotic equilibria. Redox isomers, spatially isolated orbitals, chronoamperometry, chronopotentiometry, Photoelectrochemical Solar Cell (PEC), primary coulometry and secondary coulometry, coulometric titration

**I-4162b: Inorganic Nanomaterials****(1L/W; CP:1)****Marks: 12.5**

1. Different synthetic routes: Physical, Chemical, Mechanical and electrochemical methods of nanomaterial design, Control of growth kinetics/seeding kinetics, morphology and structure, Classifications of nanosystems: 0D, 1D, 2D, 3D Nanomaterials, Size dependent properties of nanomaterials - Quantum Confinement Effects, Electronic properties and their optical behavior changes, Surface Plasmon

Resonance (SPR), Direct and Indirect Transitions: Optical phenomena in nanoscale Materials

2. Hybrid organic-inorganic nanomaterials (functionalized nanomaterials) and its wide application towards different sensor, SAMS (self-assembly of monolayers) films, Core-shell nanosystems, Bimetallic sensor probes, Janus particle, Different types of nanoclusters, Metcars and other energy harvesting materials and their applications in different areas.

3. Characterization Techniques: Differences between Light Microscope (LM) and Electron Microscope (EM), X-ray diffraction, SEM-EDX, TEM/HRTEM, DLS and electrical/thermal conductivity of nanomaterials.

4. Nanolithographic techniques, Microelectromechanical systems: fabrication, design and Applications: MEMS and NEMS devices, Electrochemical sensors and biosensors.

**PAPER: XVI-O [Organic Chemistry Special] CP: 4 Marks: 50**

**Unit– O-4161 : Amino Acids, Peptides and Proteins (2L/W; CP:2) Marks: 25**

**Protein Structure:** Amino acids (common and rare), peptides (synthetic methods including protecting groups, coupling reagents), non-protein peptides (structure of glutathione, oxytocin, vasopressin, bradykinin, enkephalins and insulin), method of elucidation of primary structure and amino acid composition of protein, secondary structures (molecular helices, pleated sheets, turns and motifs), Ramachandran diagram, prediction of secondary structural elements by circular dichroism, FTIR and Chou-Fasman method, prediction of tertiary structure by NMR, collagen triple helix: formation and stability.

Determination of molecular weight of proteins by gel filtration, electrophoresis and mass spectrometry methods. Protein denaturation and folding, thermodynamics and kinetics of protein-folding, proline *cis-trans* isomerization, molecular chaperons.

**Protein purification:** Methods of purification of proteins applying different chromatographic and gel electrophoresis techniques.

**Unit– O-4162 : Biomimetic Chemistry, Peptidomimics, Nucleic Acid-mimics,**

**Membrane-mimics**

**(2L/W; CP:2)**

**Marks: 25**

**Biomimetic Chemistry:** Basic definitions of Biomimetics, Application of Supramolecular chemistry in Biomimetic design, Relation to the designing of Drug and synthetic materials, Involvement of Organic chemistry in Biomimetics; Classifications of different biomimetic fields: Peptidomimetics, Membrane-mimetics, Nucleic Acid – mimics.

**Peptidomimetics:** Steps in peptidomimetics; Ala-scan; Backbone modification (synthesis and importance): Peptoid, Azapeptide, depsipeptide, keto-methylene etc.,  $\alpha,\beta$  and  $\gamma$ -turn-mimics; Side-chain modification (synthesis and importance); basic principles of Peptidomimetics-Drug designing.

**Membrane-mimetics:** Architecture of membrane lipids, Chemical synthesis of different membrane lipids with the variation at the Head group, Linker, glycerol-backbone and hydrophobic part. Apolar/polar ratio, Organic synthesis of functionally variable amphiphilic systems related to: DNA/gene/drug delivery systems, Soft biomaterials design; Lyotropic phases and their biophysical detection techniques (not very detailed analysis) of lipids and surfactant assemblies: NMR, Fluorescence, UV-Vis spectroscopy, Small Angle X-ray diffraction, DSC-thermal analysis, TEM, SEM, AFM –microscopy, Application of membrane mimetic in pharmaceutical applications.

**Nucleic Acid mimics:** Concept on H-bonding network between base-pairs: Hoogsteen and Watson-crick, Tripple helix, Sugar backbone modification, Base-modification, Peptide Nucleic Acid.

**PAPER: XVI-P [Physical Chemistry Special] CP: 4 Marks: 50**

**Unit–P-4161: Group Theory and its Chemical Application**

**(2L/W; CP:2) Marks: 25**

1. Quantum mechanics and group representation theory, Direct product representation. Vanishing of quantum mechanical integral, Transition probability, Selection Rules.
2. Projection operation, symmetry adapted linear combination of atomic orbitals, Construction of  $\pi$ -MO for different systems; LCAO-MO approximations Hückel theory for conjugated systems. Hybrid orbitals.
3. Symmetry and chemical reactions; Woodward –Hoffmann Rule.
4. Application of group theory to molecular vibrations, Normal modes, Vibrational transitions, IR and Raman Spectra and Selection rule.
5. Application of group theory to Ligand and crystal field theory.

**Unit– P-4162: Solid State Chemistry (2L/W; CP:2) Marks: 25**

**Fourier synthesis of a crystal structure:** Diffraction of waves by crystals; Fourier analysis; Reciprocal lattice vectors; Diffraction condition; Laue equations; Ewald construction; Brillouin zone; Reciprocal lattice to cubic lattices; Fourier analysis of the basis; Structure factor; Systematic absences; Atomic scattering factor.

**Free electron theory of metals:** Free electron gas in 1D and 3D; Fermi-Dirac distribution function; Fermi surface; Electron velocity at the Fermi surface; Density of states; Heat capacity; Electrical conductivity; Matthiessen's rule; Thermal conductivity; Wiedemann-Franz law; Hall Effect.

**Energy bands:** Nearly free electron model; Bloch functions and theorem; Kronig-Penney model; Wave equation of electron in a periodic potential.

**Junction Properties:** Metal-metal, metal-semiconductor and semiconductor-semiconductor junctions; p-n junction; Photovoltaic effect and solar cells.

**Crystal defects:** Defect sites; Schottky and Frenkel defects (derivation); Colour centres; ionic conductivity.

**Magnetic Properties:** Diamagnetism and Paramagnetism; Ferromagnetism and Antiferromagnetism; Ferrimagnetism; Curie-Weiss law; Two-sublattice model; Domain structures.

**Properties of insulators:** Piezoelectricity; Pyroelectricity; Ferroelectricity; Paraelectricity – Introductory discussion with representative examples and applications.

**Superconductivity:** Historical background; Meissner effect; Type I and Type II superconductors; Thermodynamics of superconducting transitions; BCS theory of superconductivity (salient points only); Josephson effect; Introduction to High  $T_c$  superconducting oxide materials.

## Practical Papers

(8L [2days]/W; CP: 4)

**PAPER: L-VII-A [Analytical Chemistry Special] CP: 4 Marks: 50**

Literature Review and presentation.

**PAPER: L-VII-I [Inorganic Chemistry Special] CP: 4 Marks: 50**

Literature Review and presentation

**PAPER: L-VII-O [Organic Chemistry Special] CP: 4 Marks: 50**

Project work

**PAPER: L-VII-P [Physical Chemistry Special] CP:4 Marks: 50**

A project work related to some research program, seminar & viva voce.

**PAPER: L-VIII-A [Analytical Chemistry Special] CP: 4 Marks: 50**

Project and Seminar

**PAPER: L-VIII-I [Inorganic Chemistry Special] CP: 4 Marks: 50**

Project and Seminar

**PAPER: L-VIII-O [Organic Chemistry Special] CP: 4 Marks: 50**

Seminar

**PAPER: L-VIII-P [Physical Chemistry Special] CP: 4 Marks: 50**

Computer Practical: Computer programming and its applications.