TDC (MAJOR) COURSE

First Year

SEMESTER I

PAPER M 101 Physical Chemistry (Total Marks 75)

Unit 1.1 Chemical Thermodynamics (Marks 25)

Definition of thermodynamic terms, closed, open and isolated system; surroundings, energy, heat, work, internal energy. The first law, calculation of work done during expansion of gas, thermodynamic reversibility, heat capacity, enthalpy and its significance, significance of heat and work.

State functions and differentials; variation of internal energy and enthalpy with temperature, Joule-Thomson experiment and liquefaction of gases; relation between C_p and C_V; Calculation of work done on adiabatic expansion; relation between P,V and T in adiabatic processes.

Thermochemistry- standard enthalpy changes, derivation of Hess's law and Kirchhoff's law. Relation of reaction enthalpy with changes in internal energy. Calculation of bond dissociation energies from thermochemical data.

Unit 1.2 Chemical Thermodynamics (Marks 20)

The second law, entropy changes in reversible and irreversible processes. Clausius inequality, calculation of entropy changes during various processes.

Helmholtz function and Gibb's function and the direction of spontaneous change. Thermodynamics of chemical reactions - Equilibrium constant of a reaction in terms of standard Gibb's function, dependence of equilibrium constant of temperature and pressure.

Standard entropy of a reaction and standard Gibbs function of formation. Maxwell's relations and derivation of thermodynamic equation of state; Gibb's-Helmholtz equation, variation of Gibb's function with pressure and temperature. Brief idea of partial molar quantity, chemical potential and Gibb's-Duhem equation.

Third law of thermodynamics – Nernst heat theorem.

Unit 1.3 Chemical Kinetics (Marks 20)

Concept of reaction rate and rate laws. Order and molecularity of reaction. Integrated rate expression for zero, first and second order reactions. Half-life period.

Consecutive and concurrent reaction. Steady state and rate determining step approximation. Simple problems on Steady State approximation. Experimental determination of rate and order of reaction. Temperature dependence of reaction rate and

Arrhenius plots.

Kinetics of chain reaction, H_2-Br_2 reaction, thermal decomposition of ethanol, branching and non-branching chain reaction - $H_2 + O_2 \rightarrow H_2O$ reaction. Homogeneous catalysis, acid-base catalysis. Enzyme catalysis, Michalis-Menten equation, effect of pH and temperature. Zeolites and its uses in cracking and reforming of petroleum.

Internal assessment **(Marks 10)**

PAPER M 102 Organic Chemistry (Total Marks 75)

Unit 1.4 Introduction to Organic Compounds (Marks 15)

IUPAC nomenclature of organic compounds. Hybridization of carbon in organic compounds. Bond angles, bond length and bond energies. Electron delocalization effects in organic compounds, tautomerism. Hydrogen bonding and its effect on the properties of organic molecules. Acid-base behaviour, pK_a values and factors effecting acidity/ basicity of organic compounds.

Unit 1.5 Stereoisomerism (Marks 20)

Types of steroisomerism - conformational and configurational isomers, enantiomers & diastereomers, π-distereomers- differences in physical and chemical properties of π-diastereomers. Syn/anti, cis/trans & E/Z designation. Stereomutation of π-diastereomers. Cis- trans isomerism in cycloalkanes- (upto 6- membered rings)

Enantiomers - optical activity, asymmetry, dissymmetry or chirality, racemic modification, & methods of resolution of racemic modification & projection formula- Flying-wedge formula, Fischer, Newman & Sawhorse projection. Criteria for showing optical activity, examples of optically active molecules without chiral centre, Atropisomerism.

Unit 1.5 Organic Reaction Mechanism1 (Marks 30)

Idea of driving force, activation energy, transition state, energy profile diagrams, concept of kinetic and thermodynamic control of reactions, Homolytic and heterolytic bond fission, Types of reagents-electrophiles and nucleophiles. Types of reaction intermediates- carbocations carboanions, carbenes, free radicals nitrenes arynes.

Mechanism of organic reactions

A. Addition reactions : electrophilic, nucleophilic and free radical mechanism.

   B) Substitution reactions : electrophilic, nucleophilic and free radical mechanism

B. Elimination reaction : β–elimination reaction - base catalysed and pyrolytic elimination reactions.

Internal Assessment **(Marks 10)**

PAPER M 103 Practical (Total Marks 50)

A. **General Experiment** *(any one of the following to be done in Exam)* **(Marks 30)**

1. To determine the solubility of a given salt at different temperatures and to plot solubility curve.

2. To determine water of crystallization of hydrated salt by ignition and weighing.

3. Determinations of the concentrations of sodium carbonate and sodium hydroxide in a given mixture.

4. To study the kinetics of the reaction between H_2O_2 and iodide ion.

5. Kinetics of Clock reaction between $S_2O_3^{2-}$ and HCl.

6. Study the adsorption of oxalic acid on activated charcoal

7. Estimation acetic acid in vinegar by conductometry.

8. Column chromatographic/ TLC separation of pigments from green leaves.

9. Separation of a mixture of benzoic acid, 2-naphthol and 1,4-dimethoxybenzene by solvent extraction and identification of their functional groups.

10. Paper chromatographic separation and identification of sugars.

B. **Sessional (Marks 10)**

C. **Viva (Marks 10)**

Semester II

PAPER M 201 Physical Chemistry (Total Marks 75)

Unit 2.1 Gaseous State (Marks 20)

Deviations from ideal behaviour, van der Waals equation of state, Virial equation of state, Critical phenomena, Equation of Corresponding States. Kinetic theory of gases, distribution of molecular speeds. Mean, root mean square and most probable speeds, Collision cross section, Mean free path.

Transport properties, Flux and Fick's law of diffusion, thermal conductivity and viscosity of gas from kinetic theory.

Degrees of freedom, Principle of equipartition of energy. Molecular basis of heat capacity.

Unit 2.2 Liquid State (Marks 10)

Structure of liquid (qualitative treatment) – structure of liquid water and ice. Physical properties of liquid – determination of vapour pressure, capillary action, determination of surface tension and viscosity. Refractive index of liquids. Elementary idea of structure, physicalproperties and uses of liquid crystals.

Unit 2.3 Colligative Properties (Marks 10)

Thermodynamic treatment of colligative properties. Ostwald's law and Henry's law. Definition of colligative property, ebullioscopy, cryoscopy, calculations based on relative lowering of vapour pressure and solubility of an ideal solute. Osmosis, van't Hoff's equation. Abnormal colligative properties.

Real solution – activity, activity coefficient.

Unit 2.4 Electrochemistry (Marks 25)

Ion transport and conductivity. Molar conductance and its temperature dependence. Kohlrausch's law. Mobility of ions and conductivity. Transport number of ions and its determination.

Debye-Huckel-Onsager equation, Stokes-Einstein relation. Activity of ions. Debye-Huckel theory (elementary ideas) of strong electrolytes. Ionic strength of solutions.

Electrochemical cells, measurement of emf, electrode potenmtial, sign convention. Different types of electrodes, the calomel electrode. Nernst equation, the electrochemical potential and its measurement. Equilibrium constants and activity coefficients from standard electrode potentials.

Concentration cell with and without transference, Galvanic cells, Fuel cell, Batteries and Dry cell. Corrosin.

Strong and weak electrolytes, dissociation equilibria of weal electrolytes. Ostwald's dilution law. pK of acids and bases. Buffer solution. Henderson Hasselbach equation. Buffer action.

Internal Assessment **(Marks 10)**

PAPER M 202 Organic Chemistry (Total Marks 75)

Unit 2.5 Stereoisomerism (**Marks 10)**

Conformation of molecules - ethane, butane, cyclohexane, relative stability of conformers.

Concept of topocity and prostereoisomerism, criteria of establishing topocity of groups, atoms and faces, designation of stereoheterotopic atoms, groups and faces.

Unit 2.6 Reaction Mechanism 2
(Marks 15)

a) Mechanism of electrophilic aromatic substitution. Directive influence of groups, activation and deactivation of aromatic rings, o/p ratio, mechanism to be given with examples.

b) Mechanism of nucleophilic aromatic substitution. Intermediate complex mechanism, benzyne mechanism. Directive influences in benzyne mechanism. Cine substitution, methods of trapping benzyne intermediates.

Unit 2.7 Organic Compounds (Marks 40)

I. Aliphatic Compounds: General methods of preparation, physical properties, reactions and

functional group transformation of

a. Saturated and unsaturated hydrocarbons
b. Alkyl halides
c. Primary, secondary and tertiary alcohols, diols, triols
d. Carbonyl compounds
e. Carboxylic acids
f. Nitro compounds, and
g. Primary, secondary and tertiary amines

II. Aromatic Compounds: General methods of preparation, Physical properties, Reactions and

functional group transformation of aromatic (benzene) compounds.

h. Benzenes and arenes
i. Aromatic Halogen compounds
c. Phenols and benzyl alcohols
d. Aromatic carbonyl compounds

e) Aromatic carboxylic acids

f) Aromatic nitro compounds

g) Aromatic amines and

h) Polynuclear hydrocarbons-naphthalene, anthracene.

Internal Assessment **(Marks 10)**

PAPER M 203 Organic Practical (Total Marks 50)

A. Qualitative Organic Analysis (**Marks 30)**

Analysis of an organic compound & identification by

a) Detection of N, S, Halogens b) Test for functional groups

c) Solubility, melting point, boiling point

d) Preparation of a derivative and determination of its melting point

(Distribution of Marks : Detection of elements – 5, Test for Functional group – 10, solubility, aromaticity, unsaturation test, mp/bp – 8, Preparation of derivative & mp – 5, Identification – 2)

B. Sessional **(Marks 10)**

C. Viva **(Marks 10)**

Second Year

Semester III

PAPER M 301 Structure and Bonding (Total Marks 75)

Unit 3.1 Atomic Structure (Marks 40)

Learning Structure of hydrogen-like atoms and their representation in quantum mechanical terms. Basic quantum mechanical ideas and principles leading to atomic structure (outline only without details) :

a) Particle character of radiation - black body radiation phenomenon - Planck's hypothesis : Postulates and explanation for black body radiation.

b) Wave character of particles-electron diffraction.

c) Discrete nature of energy levels of atomic and molecular systems, line spectra of atoms (e.g., hydrogen) and molecules (e.g.N_2O).matter-de Broglie hypothesis.

d) Dual nature of matter-de Broglie hypothesis. e) The defining limit of classical mechanics-the uncertainty principle.

f) Definition of micro and macro particles.

g) Necessity of quantum mechanical equation.

h) Schrodinger equation-statement and identity of terms. Energy eigenvalues-expression alone. Energy eigenfunctions: Setting up of expressions of radial(R) and angular(Y) parts for $1s,2s,2p_o,2p_{+1},2p_{-1},2p_x,2p_y,2p_z$ orbital, Born interpretation of the wave functions, Orbital concept-one electron wave functions, Plots of and ψ^2 for $1s,2s,2p,2p_x,2p_y,2p_z,3d_{xy},3d_{zx}$ orbital. n,l,m quantum numbers-origin and significance(outline only).

i) The concept of spin and spin quantum numbers (outline only).Many electron atoms. Electron repulsion in the He atom. Pauli's exclusion principle. Aufbau principle and electron configuration of many electron atoms.

j) Effective nuclear charge-shielding and penetration effects. Electron Configuration of atoms.

Unit 3. 2 Chemical Bonding I
(Marks 25)

Lewis electron pair bond. Valence bond approach to bonding in diatomic molecules-outline of concept of overlap (HF and H_2). Resonance and resonance energy in HF and benzene. Bond moments and dipole moments (outline with simple pictorial representation). Percent ionic character of HCl and HF bonds. Formal charges on atoms in molecules. Concept of electro negativity -explanation of molecular properties on the basis of electro negativity.

Internal Assessment **(Marks 10)**

PAPER M 302 (Total Marks 75)

Unit 3.3 Chemical Bonding II (Marks 20)

Shapes of molecules- VSEPR theory, hybrid orbital and hybridization in polyatomic molecules-influence of hybridization on bond length, bond angle and other properties of molecules including shapes and dipole moments. Effects of structure on molecular properties- steric effects and electronic effects.

Unit 3.4 Chemical Bonding III (Marks 25)

Molecular orbital theory of homonuclear diatomic molecules (N_2, O_2, F_2,CO, NO etc).Graphical representation of angular parts of the wave function(H_2^+ molecule ion).Energy levels, electronic configuration of ground states of diatomic molecules.

Setting up of the wave functions and energy level diagrams for H_2 molecules without calculations. Multicentre bonding(diborane);MOs of simple triatomic systems (BeH_2,H_2O,NO_2);Multiple bonding, orbital picture and energy of ethane,ethyne and benzene; Huckel' s aromaticity rule.Delocalisition vs. Resonance; bond energy; bond length and covalent radii. Bonding in metals (band theory); properties consequent from Band theory.

Unit 3.5 Ionic Bonds and Solids (Marks 20)

Types of solids, macroscopic properties of solids, properties of ionic compounds; types of unit cells; crystal lattices and Miller indices; crystal system and Bravais lattices.Closed packed structures, ionic radii; radius ratio and structures; Spinel and Perovskite structures, Lattice energy of ionic solids; Born- Haber cycle-calculations; Covalent character of ionic bonds-Fajan's rules of polarization. Inter-molecular forces-dipole moment and molecular polarisability. Molecular solids; Hydrogen bonding and its effect on physical properties.

Internal Assessment **(Marks 10)**

PAPER M 303 Practical
(Total Marks 50)

A. Qualitative Inorganic Analysis (Marks 30)

Analysis of a mixture of salts containing total of five cations and anions including insoluble salts and interfering anions.

Marks distribution :

1. Physical properties and solubility 2 marks
2. Preliminary Dry tests 4 marks
3. Dry test for acid radicals 4 marks
4. Wet test for acid radical 4 marks
5. Confirmatory test 2 marks
6. Group analysis 4 marks
7. Conclusion and remarks (2x5=10) 10 marks

B. Sessional (Marks 10)

C. Viva (Marks 10)

Semester IV

PAPER M 401 (Total Marks 75)

Unit 4.1 Properties of Inorganic Compounds (Marks 25)

Groupwise and periodwise trends in physical and chemical properties of elements and their compounds with illustrative examples from Groups 1, 2, and 13-17. The following should be emphasized, explaining the factors affecting these trends-

(a) Electronic configuration, effective nuclear charge, Slater's rule, size of atoms, ions and atomic orbital.

(b) Ionization energy and electron affinity of atoms.

(c) Tendency for homo and hetero catenation, the energy of M-M, M-O and M-X bonds

(M=element, X=halogen).

(d) Tendency to use vacant d-orbital and electropositive character of metals.

(e) Electro negativity of elements.

(f) Melting point and boiling point of elements and their compounds.

(g) Solubility of salts and molecules in water.

(h) Relative acid –base strength of Lewis and protonic acids with reference to oxides,

hydroxides and oxoacids.

(i) Electrode potentials and redox behaviour in aqueous solutions.

Unit 4.2 Chemistry of Non-transition Elements I (Marks 25)

Polarizing power of cations, Polarisability of anions and consequences of Fajan's rules, the concept of chemical hardness and the theory and applications of Pearson's HSAB concept.

The Latimer diagram and Frost diagram and their uses.

Non aqueous solvents : liquid ammonia, liquid sulphur dioxide, liquid HF and liquid N_2O_4.

Preparation, properties, bonding and structure of the following (excepting where specific aspects have been mentioned):

a. Ortho and Para hydrogen, hydrates, clathrates and inclusion compounds, binary metallic hydrides.

b. Diborane and higher boron hydrides.

c. Allotropes of carbon (including fullerenes), graphite, intercalation compounds,

carbides, cyanogens, oxides and oxoacids of carbon.

Unit 4.3 Chemistry of Non-transition Elements II (Marks 15)

a. Allotropes of phosphorous, Hydrides, oxides and oxoacids of nitrogen and phosphorous, Hydrazine, Hydroxylamine and hydrogen azide, clinical use of NO and N_2O.

b. Super oxide and oxygen fluorides, Allotropes of sulphur, halides, oxides, hydrides, oxoacids and per acids of sulphur, mechanism of formation and depletion of ozone layer.

Internal Assessment **(Marks 10)**

PAPER M 402 (Total Marks 75)

Unit 4.4 Chemistry of Non-transition Elements (Marks 15)

a. Interhalogen compounds, polyhalides, pseudo halogen, oxides and oxoacids of halogens.

b. Noble gas compounds-xenon oxides and fluorides.

c. Inorganic chains, ring and cages: Silicate, Aluminosilicates, zeolites, silicones, Borazine, Phosphazine, S_4N_4, P_4, P_4O_6, P_4O_{10}, boron cage compounds, carboranes and metallocarboranes.

Unit 4.5 Chemistry of Metals (Marks 25)

Bonding in metals, physical and chemical properties of metals, important alloys and intermetallic compounds. Occurrence and principles of extraction of Ni, Cr, Mn, Au, V and Mo. Physical and chemical properties of ionic compounds of alkali metals, alkaline earth metals and aluminium. Allotropes of tin, Inert pair effect in Sn, Pb and Tl, structure and properties of oxides, hydroxides and halides. Coordination compounds of Sn, Pb, As and Se. Zn, Cd, Hg: Stereochemistry of compounds, the mercurous ion, divalent compounds, coordination complexes.

Unit 4.6 Transition Metals (Marks 25)

Electronic configuration and general periodic trends, comparative study of first transition series elements, preparation, properties and reactivity of oxides, hydroxides and halides of V-Cu.

Trends in physical and chemical properties of second and third transition series in comparison to the first, study of oxides and halides of Au,Ag,Mo,Ru,Rh,Ir,Pd and Pt.

Coordination Compounds: Werner's theory, structural and stereo isomers of complex compounds, survey of different types of ligands, IUPAC nomenclature of coordination compounds. Preparation, structure, bonding and reactivity of complexes containing the following as one of the ligands: CO, N_2, CN^-, O_2, CH_3COO^-, $C_2O_4^{2-}$, NH_3, en, acac.

Internal Assessment **(Marks 10)**

PAPER M 403 Practical (Total Marks 50)

A. General Chemistry Experiments (Marks 10)

a. To determine the water of crystallization of green vitriol by titration with 0.1N $KMnO_4$ solution.

b. To determine the hardness of water by EDTA titration.

c. To determine temporary and permanent hardness of water by EDTA titration.

B. Inorganic Preparation (Marks 20)

a. Preparation of the following:

1 Chrome alum and crystallization

2 Tetra mine Cu(II) sulphate

3 $Cu(glycinate)_2$

4 Hexammine Ni(II)chloride

5 Potassium trioxalato ferrate(III)

6 Potassium trioxalato chromate(III)

7 Cu(thiourea)complex

8 Mohr's salt

b. Characterization of the compound prepared

Students should recrystallize the product and verify presence of anions and cations by

qualitative analysis.

C. Sessional (Marks 10)

D. Viva (Marks 10)

Third Year

Semester V

PAPER M 501 : Quantum Chemistry (Total Marks 75)

Unit 5.1 Quantum Theory Marks 30

Review of experiments leading to the idea of quantization –

(a). Black body radiation – Planck's hypothesis

(b). Photoelectric effect – Einstein's explanation

(c). Compton effect

Electron diffraction, de Broglie hypothesis, Heisenberg's uncertainty principle. Postulates of Quantum mechanics.

Wave functions, Operators, Eigen functions and eigen values, the Schrodinger postulates of operator transforms and the wave equation boundary conditions, normalization of the wave functions, expectation values. Interpretation of the wave function – orthogonal and orthonormal wave functions.

Model systems – particle in 1D and 3D boxes – particle in a ring, harmonic oscillator and rigid rotator (detailed mathematical treatment not necessary) : coordinate systems – construction of

Hamiltonian – potential function leading to potential energy term – Schrodinger equation, outline of solution, energy expression, wave functions, quantum numbers. Special features like degeneracy, energy level diagrams, plot of wave functions and their squares vs displacement from origin, zero point energy, quantum mechanical tunneling, force constant and bond strength (for harmonic oscillator), moment of inertia in 3D, angular momentum, space quantization of angular momentum (for rigid rotator).

Qualitative discussion of all these topics.

Unit 5.2 Atomic Structure Marks 20

The Hamiltonian and Schrodinger equation for hydrogen atom, energy levels and quantum numbers, the radial and the angular part of the wave function, construction of two dimensional plots of probability density and calculation of radial probability functions. The orbitals of hydrogen and hydrogen-like atmos, contour diagrams of electron density. Stern-Gerlach experiment, electron spin and spin quantum number – spin orbitals. Electron configuration of many electron atoms, Pauli's exclusion principle – illustration by He atom using wave functions.

Spin-orbit interactions, Russel-Saunder's coupling, Term symbols. Effect of magnetic

field on energy levels. Hund's rule.

Unit 5.3 The Nature of Chemical Bond Marks 15

Schrodinger equation for a molecule, Born-Oppenheimer approximation. LCAO-MO theory as applied to H_2^+ and H_2 - drawback of MO theory. MO energy level diagram of homonuclear (O_2, N_2) and heteronuclear (HF, LiF, CO) diatomic molecules. Heitler-London theory – wave function and potential energy curve of H_2. Concept of resonance and hybridisation from VB theory. Term symbols of diatomic molecules. Huckel theory for ethene and benzene.

Internal Assessment **(Marks 10)**

PAPER M 502 Physical Chemistry (Total Marks 75)

Unit 5.4 Molecular Reaction Dynamics (Marks 15)

Collision theory, Activated complex theory; Erying equation – thermodynamic formulation. Theory of unimolecular reactions (Lindemann) – dynamic molecular collisions – potential energy surfaces – Molecular beam technique and results of molecular beam studies. Reactions in solution, Bronsted- Bjerrum equation, Kintic salt effect. Introduction to lasers, flash photolysis.

Unit 5.5 Photochemistry (Marks 15)

Laws of photochemical equivalence, Quantum yield, chemical actinometry Kinetics of H_2-Br_2 , H_2-Cl_2 reactions, Dissociation of HI, Photostationary equilibrium, Dimerisation of anthracene.

Luminescence phenomenon – fluorescence, phosphorescence, Jablonski diagram, Photosensitised reactions, Quenching of fluorescence. Chemi and bio luminescence.

Photochemistry of air and air pollution.

Unit 5.6 Phase Equilibria (Marks 20)

Definition of phase, meaning of components and degrees of freedom. Derivation of phase rule. Phase diagram of one component system (water). Phase diagram of two component system – eutectics, congruent and incongruent melting points, solid solutions.

Interpretation of liquid-vapour, liquid-liquid and liquid-solid phase diagrams. Distillation of partially miscible liquids.

Clausius Clapeyron equation for different phases. Systems of variable composition, partial molar quantities, Gibbs Duhem equation, Thermodynamics of mixing.

Chemical potential, chemical potential of a component in an ideal mixture – fugacity,

activity coefficients. Dependence of chemical potential on temperature and pressure.

Unit 5.7 Surface Chemistry (Marks 15)

Introduction to solid surfaces, adsorption on surfaces – physisorption and chemisorption. Adsorption isotherms – Langmuir, Freundlich, BET equation. Determination of surface area, Catalytic activity at surface with examples.

Concept of surface excess, Gibbs equation, surface pressure and surface spreading.

Internal Assessment **(Marks 10)**

PAPER M 503 Organic Chemistry (Total Marks 75)

Unit 5.8 Organic Reaction Mechanisms (Marks 35)

A. **Molecular Rearrangements of the types**

Nucleophilic or anionotropic : Whitmore 1,2 Shift, Wagner-Meerwein, Wolff, Hofmann, Lossen, Curtius, Schmidt, Beckman, Favorskii, Benzil- benzilic acid, Baeyer Villiger

Free radical : Wittig

Electrophilic or cationotropic : Pinacol

Special : Fries rearrangement (aromatic electrophilic substitution)

Stevens (ion pairs in solvent cage/ radical pair)

B. **Oxidation - reduction : common oxidizing and reducing agents.**

i) Direct electron transfer: Clemmensen (Nakabayashi mechanism)

ii) Hydride transfer

iii) Hydrogen Atom Transfer: Bouveault-Blanc

iv) Formation of ester intermediate: oxidation by dichromate, permanganate, etc.

v) Displacement mechanism.

vi) Addition- elimination.

Oxidizing agents : Chromium oxide, selenium dioxide, Chromyl chloride, PCC, and Lead tetraacetate.

Catalytic hydrogenation (Pd, Pt, Raney Ni). Reduction by LAH, Sodium Borohydride and metals (Birch). Reduction of nitro group under various condition. Selective reduction- Rosenmund reduction, Lindlars catalyst.

C. **Pericyclic Reactions**

Definition and examples of 2+2 and 2+4 cycloadditions. The conservation of orbital symmetry. Woodward Hoffman rules. Diels Alder reaction, 1,3 Dipolar Cycloaddition. Sigmatopic rearrangements-Cope and Claisen rearrangements. Electrocyclic reactions- HOMO-LUMO approach.

Unit 5.9 Polynuclear Aromatics, Nitro and amino compounds, Organo S and organo P Compounds, Active methylene compounds and Heterocyclic compounds (Marks 30)

Polynuclear aromatic hydrocarbons

Structure, bonding, properties and reactivity of naphthalene and its derivatives. Anthracene, phenanthrene

and anthraquinone-important methods of synthesis.

Nitro and amino compounds

Synthesis, physical properties and reactivity of nitroalkanes, alkyl nitrates, alkyl nitriles, isonitriles and

aromatic nitro compounds. Synthesis, reactions and basicity of aliphatic and aromatic amines.

Diazotization and its mechanism. Distinction between primary, secondary and tertiary amines,

Quarternary ammonium salts, Hofmann exhaustive methylation and Hofmann degradation of amines.

Organo S and organo P compounds

Synthesis and reactions of thiols, thioethers and aliphatic sulphonic acids. Phosphines, Phosphorous esters

and phosphorous ylides- Wittig reaction.

Active methylene compounds

The active methylene groups, synthesis of compounds containing active methylene groups (Ethylacetoacetate, Diethylmalonate and cynaoacetic ester) and their use in organic synthesis.

Heterocyclic compounds

IUPAC nomenclature, Synthesis, structure and bonding, properties (basicity, aromaticity) and reactions of pyrrole, furan, thiophene, pyridine, indole and quinoline.

Internal Assessment **(Marks 10)**

PAPER M 504 Inorganic Chemistry (Total Marks 75)

Unit 5.10 Bonding in Coordination Compounds (Marks 25)

Symmetry elements and Symmetry operation, Point group classification, Symmetry of octahedron, tetrahedron and square planar complexes, Structure and symmetry of inorganic compounds(coordination 2-8), Shape and symmetry of s,p and d orbital.

Crystal field theory, factors affecting 10 Dq value, crystal field stabilization energy, Magnetic properties from crystal field theory, high spin and low spin complexes, structural and thermodynamic affects of orbital splitting, octahedral coordination in Spinels. Adjusted crystal field (or Ligand field) theory, Molecular orbital theory of octahedral complexes (without and with p bonding).

Metal-metal bonding and quadruple bonds.

Unit 5.11 Organometallic Compounds (Marks 30)

Synthesis, structure and bonding of complexes with olefins, acetylene, allyl, cyclopentadiene and arenas. IUPAC nomenclature. Effective Atomic number rule, Transition metal to carbon sigma bonds.

Homogeneous catalysis by transition metal complexes (isomerzation, hydrogenation, hydroformylation and Ziegler-Natta Polymerization).

Synthesis and structure of organomettalic compounds of Sn and Pb, Organometallic compounds of Zn, Cd and Hg.

Unit 5.12 Bioinorganic Chemistry I (Marks 10)

Essential and trace elements and their biological role, Importance of Na/K salts and calcium in biology.

Uptake and storage of iron, Introduction to the structure and function of hemoglobin, Synthetic dioxygen carriers, Dioxygen toxicity.

Internal Assessment **(Marks 10)**

PAPER M 505 Practical (Total Marks 75)

A. Inorganic Quantitative Analysis (Marks 40)

Estimation of inorganic ions by volumetric, complexometric, gravimetric, redox and precipitation methods.

The following one-component systems should be estimated first: Cu, Fe, Ca, Mg, Ni, Cl and SO_4^{2-}. This should be followed by separation and estimation of individual ions in two-component systems of-

a. Cu and Fe

b. Fe and Ca

c. Ca and Mg

d. Cu and Ni and

e. Cl^- and SO_4^{2-}.

(Any one of the above mixtures will be given for estimation in examination. Determination of marks: Preparation of standard solution and standardization 10 marks. Separation of components 5 marks, Completion of the experiment 10 marks, and Results 25 marks.)

B. Chromatographic separation of cations by paper/TLC (Marks 15)

Colorimetric estimation of Cu^{2+}.

(Any one of these two experiments is to be done in the examination)

C. Sessional (Marks 10)

D. Viva (Marks 10)

PAPER 506 Practical (Total Marks 75)

A. Organic preparation (Marks 25)

Any one of the following will have to be done in the examination :

a). Acetylation : Preparation of - acetanilide from aniline and aspirin from salicylic acid.

b). Benzoylation : Preparation of benzanilide from aniline.

c). Nitration : Preparation of - *m*-dinitrobenzene and *p*-nitroacetanilide from acetanilide.

d). Halogenation : Preparation of *p*-bromoacetanilide from acetanilide and 2,4,6-

tribromophenol from phenol.

e). Diazo-coupling : Preparation of methyl orange.

f). Oxidation : Preparation of benzyl from benzoin.

g). Reduction : Preparation of *m*-nitroaniline from *m*-dinitrobenzene.

(Distribution of marks : Yield & Quality of the compound – 10, Recrystallisation & melting

point – 10, completion – 5.)

C. Organic quantitative analysis (Marks 30)

Any one of the following experiments will be asked in the examination :

a). Determination of the equivalent mass of a carboxylic acid by direct titration method.

b). Determination of saponification equivalent of an ester.

c). Determination of amount of glucose by titration with Fehling solution.

d). Estimation of urea by hypobromite method.

(Disttribution of Marks : Theory – 4, Preparation of standard solution & standardization – 6,

completion – 5, Result – 15.)

D. Sessional (Marks 10)

E. Viva (Marks 10)

Semester VI

PAPER M 601 Spectroscopy (Total Marks 75)

Unit 6.1 Introduction to Spectroscopy (Marks 10)

The nature of electromagnetic radiation. The regions of spectrum. Mechanism of interaction of electromagnetic radiation with matter. Absorption and emission spectroscopy. Basic elements of practical spectroscopy. Representation of spectrum – the width of spectral line. Intensity of spectral lines. Selection rules for various transitions. The Beer-Lambert law, molar absorption coefficient and absorbance. Molecular motion

and energy – degree of freedom. Moment of inertia.

Unit 6.2 Rotational, Vibrational and Raman Spectroscopy (Marks 20)

Rotational spectra of diatomic molecules – rigid rotator concept – determination of bond length – effect of isotopic substitution – spectra of non-rigid rotator. Vibrational spectra of diatomic molecules – harmonic and anharmonic oscillator model – Morse potential - calculation of force constants – effect of isotope - vibrations of polyatomic molecules, overtone and combination bands (H_2O, CO_2). Diatomic vibrating rotor – vibration rotation spectrum of CO. Principle of Raman spectroscopy – rotational and vibrational Raman spectra of linear molecules – rule of mutual exclusion.

Structure elucidation by IR spectroscopy – finger print region and group frequencies – effect of hydrogen bonding (alcohol, keto-enol) and coordination to metal.

Unit 6.3 Electronic spectroscopy (Marks 15)

Electronic transitions and selection rule - spectrum of atomic hydrogen – fine structure, spectra of H-like atoms.

Electronic transitions in diatomic molecules – Selection rule - Born Oppenheimer approximation – vibrational coarse structure - Frank Condon principle – electronic transitions in polyatomic molecules.

Structure elucidation by electronic spectroscopy – chromophore, auxochrome – absorption due to ethylenic chromophore – Woodward's rule. Electronic transitions in conjugated polyenes from particle in a box model. Effect of solvents on electronic transition, quantitative estimation by spectrophotometry.

Introduction to photoelectron spectroscopy and its applications in simple diatomic molecules.

Unit 6.4 Spin resonance spectroscopy (Marks 10)

Interaction between spin and magnetic field – Nuclear spin – Nuclear magnetic resonance spectroscopy – ^{1}H NMR – presentation of the spectrum - chemical shift and its unit – chemical shifts for simple organic molecules (alkane, alkene, alkyne, arenas, aldehydes, carboxylic acids and esters). Spin-spin coupling and high resolution ^{1}H NMR spectra of ethanol, ethyl benzoate, 2-iodopropane, cyanohydrin.

Basic concept of electron spin resonance spectroscopy – presentation of the spectrum – hyperfine structure – esr of H- atom , deuterium atom.

Unit 6.4 Mass spectroscopy (Marks 10)

Mass spectroscopy - principle – idea of mass spectrometer – fragmentation pattern – nitrogen rule - simple applications in structure elucidation (butane, ethane, acetone) – McLafferty rearrangement (hexanoic acid, pentanal).

Internal Assessment **(Marks 10)**

PAPER M 602 Physical Chemistry (Total Marks 75)

Unit 6.4 Solid State (Marks 20)

Laws of Crystallography, Miller indices, Symmetry in solids, Bragg's law, Introduction to X-ray crystallography and determination of structure of solids. Packing in solid – octahedral hole, tetrahedral hole, radius ratio.

Dislocation in solids – Schottky and Frenkel defects, Dielectric property of solids, Concept of piezo and ferro electricity. Electrical property of solids (conductor, insulator, n type and p type semiconductors. Super conducting materials. Magnetic properties of solids (dia-, para-, ferro- and antiferro magnetism).

Uni 6.5 Macromolecules and Colloids (Marks 20)

Colloids : Definition, sols, lyophobic colloids. Structure, surface and stability of colloids. Sruface-active agents, micelle formation, critical micellar concentration, electrical double layer and Electrokinetic phenomena.

Molecular weight of macromolecules – number average and mass average molecular weight. Determination of molecular weight of macromolecules. Condensation and addition polymerization. Introduction to polymerization kinetics.

Unit 6.6 Statistical Thermodynamics (Marks 20)

Molecular energy levels and Boltzmann distribution, molecular partition function and its significance. Translational, rotational anf vibrational partition functions. Molecular significance of heat and work. Statistical thermodynamics of monatomic and diatomic gases. Applications of statistical thermodynamics for calculation of heat capacity, residual entropy and equilibrium constants.

Unit 6.7 Data Analysis (Marks 5)

Types of errors. Propagation of errors. Accuracy and Precision. Significant figures. Least square analysis. Average standard deviation. Uncertainty in the measurement of physical quantities.

Internal Assessment **(Marks 10)**

PAPER M 603 Organic Chemistry (Total Marks 75)

Unit 6.8 Organic Photochemistry, Polymers and Fibres (Marks 20)

Theory of photochemistry: photophysical processes, electronic excitation, excited states, Jablonski diagram, Franck-Condon Principles. Fluorescence and phosphorescence, ET process, photosensitizers, Einstein's law of photochemical equivalence, quantum yield.

Typical photoreactions: Photoreaction of benzophenone, photolytic reactions of ketones,

Norrish type I & Norrish type II reactions, *cis-trans* isomerisation and dimerisation, cycloaddition of olefins.

Polymers and fibres: Addition and condensation polymers, Preparation of vinyl polymers, synthesis of terylene, nylon, Elastomers-natural rubber, synthetic rubber, Urea formaldehyde resins.

Biopolymers: Polysaccharides-structure of cellulose and starch, lignins, Proteins-polypeptides and polynucleotides.

Unit 6.9 Biochemistry (Marks 20)

Structure of cell: lipids and structure of cell membrane; membrane transport

Basic molecules of living systems and their structures-Carbohydrates, proteins, nucleic acids.

Amino acids, peptides and polypeptides: Primary, secondary, tertiary and quarternary structure of proteins. Structure and functions of hemoglobin and and myoglobin.

Enzymes and their function as catalysts: chymotrypsin and lisozyme. Metalloenzymes, carboxypeptidase and peptide hydrolysis. Coenzymes and vitamins.

Structure and hydrogen bonding in purines and pyrimidines.

Structure of nucleotides and nucleosides. Structure of RNA and DNA.

Gene and genetic code: biosynthesis of DNA (replication), RNA (transcription) and proteins (translation)

Fundamentals of biological energy production-Glycolysis, Krebs cycle, Photosynthesis, respiration, oxidative phosphorylation and ATP synthesis.

Unit 6.10 Natural Products and Medicinal Chemistry (Marks 25)

Terpenes: Definition, isolation and classification, isoprene rule. Isolation, structure determination, and synthesis of important terpene- citral.

Alkaloids: nicotine only. Definition, classification and functions of hormones.

Definition and classification of carbohydrates. Structure, configuration and reactions of glucose.

Drugs-physiological effect of their structure. Classification Chiral drugs and asymmetric synthesis. Antibiotics and their action. Anticancer and antimalarial drugs. Immunity and AIDS.

Sulpha drugs- their mechanism of action. Preparation of aspirin, quinine, chloroquin, paracetamol, phenacitin, sulphanilamide and other sulpha drugs.

Cisplatin

Internal Assesment **(Marks 10)**

PAPER M 604 Inorganic Chemistry (Total marks 75)

Unit 6.10 Spectra of coordination compounds (Marks 25)

Free ion terms and their splitting in octahedral symmetry, Orgel diagram, Laporte selection rule, vibrionic coupling and colour of complexes, Electronic spectra of $M(H_2O)_6^{n+}$ complex ions.

Principles of colorimetric determination of metals, Thermodynamic stability, Stepwise formation constants, the chelate effect, kinetic lability and inertness, Mechanism of ligand displacement reactions in octahedral and square planar complexes, Determination of composition of ionic compounds by conductometry, Theory of redox and complexometric titrations.

Unit 6.11 Bioinorganic Chemistry II (Marks 15)

Metalloproteins and their role in photosynthesis, respiration, Nitrogen fixation (comparison with Haber's process).

Toxicity due to Metal ions (Fe, Cu, Al, Hg, Pb, Cd, As). The effect of gases and polluted environments (CO_2, CO, NO, SO_2, CN, nitrate, nitrite and phosphate)

Importance of metal salts in diet, diagnosis, chemotherapy and as medicines.

Unit 6.12 Nuclear Chemistry, Lanthanides and Actinides (Marks 25)

Physical properties of the proton and the neutron, Structure of the nucleus, Mass defect and binding energy, Radioactive decay and equilibrium, Nuclear reaction Q value, nuclear cross sections.

Theory of radioactive disintegration, Rates of disintegration, the radiochemical series, Transmutation of elements and artificial radioactivity, Fission and fusion, Nuclear reactors and their use, Methods of measurement of radioactivity.

Isotopes of elements (discovery, atomic weights), Methods of separation of isotopes, Application of isotopes (Tracer technique, neutron activation analysis, radiocarbon dating).

Lanthanides: Electronic configuration, stability of oxidation states, Lanthanide contraction, Coordination compounds, Separation of lanthanides.

Actinides: Discovery, electronic configuration, oxidation states, magnetic properties, Comparison with lanthanides.

Internal Assesment **(Marks 10)**

PAPER M 605 Practical (Total Marks 75)

Physical Chemistry Experiments :

At least 10 experiments are to be performed from the list of experiments given below:

1. To determine the cooefficient of viscocity of a given liquid by Ostwald viscometer.

2. To determine the composition of a given mixture by viscosity method.

3. To determine the surface tension of a liquid by stalagmometer.

4. To determine the composition of a given mixture by surface tension method.

5. To determine the mutual solubility curve of phenol and water.

6. To determine the molecular mass of a volatile liquid by Victor Meyer's method

7. To determine the specific rotation of an optically active substance by polarometric method.

8. To determine the specific reaction rate of hydrolysis of methylacetate catalyzed by hydrogen

   ions at room temperature

9. To find the rate of decomposition of H_2O_2 catalyzed by Fe^{3+} ions.

10. To test the validity of Beer-Lambert's law using colorimeter.

11. To study the rate of acid catalyzed iodination of acetone.

12. To obtain Freundlich isotherm for adsorption of oxalic acid on activated charcoal.

13. To study the distribution of iodine between CCl_4 and water.

14. To prepare arsenous sulphide sol and compare the precipating power of mono, di and trivalent

   cations.

15. To verify Debye, Huckel, Onsagar equation for sodium chloride.

16. Conductometric titration HCl vs NaOH, Oxalic acid vs NaOH, Acetic acid vs NaOH.

17. Potentiometric titration HCl vs NaOH, Oxalic acid vs NaOH, Acetic acid vs NaOH.

Distribution of marks :

Theory : Marks 10

Presentation of results including tabulation of data ,

drawing of graphs, systematic reporting : Marks 25

Completion : Marks 10

Results : Marks 10

Sessional : Marks 10

Viva : Marks 10

PAPER M 606 Project work (6 months) (Total Marks 75)

Investigation of a particular assignment given to individual student. Different project to be given to each student.

Distribution of marks:

1. Internal to be given by a Board of examiners which will include all the teachers of the Department. 25 marks

2. External 25 marks

3. Presentation of the project by the student (external + Board of examiners) 15 marks

4. Internal (to be given by the supervisor only) 10 marks

TDC (GENERAL) COURSE

First Year