Chemistry

UG (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 PV 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 Gibbs 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

TDC (MAJOR) COURSE

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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 Heary'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
e. 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 $1s,2s,2p,2p_x,2p_y,2p_z,3d_{xy},3d_{x^2}$ 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 1 (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, 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)