Post Graduate Syllabus in Chemistry for
Proposed Four Semester M.Sc. Course (2 Years) under
Credit Based Semester System (CBSS)
DEPARTMENT OF CHEMISTRY
NORTH LAKHIMPUR COLLEGE (AUTONOMOUS)

Proposed Structure of the syllabus in terms of Number of papers, Credits and Marks

Semester	Paper/LTP	Title	Credit	Marks	Semester Total Marks	Semester Total Credit
SEM-I	CT-3-CHM-101	Inorganic Chemistry	3	60	400	20 (TH=15 PR=05)
	CT-3-CHM-102	Organic Chemistry	3	60		
	CT-3-CHM-103	Physical Chemistry	3	60		
	CT-3-CHM-104	Quantum Chemistry I	3	60		
	CT-3-CHM-105	Spectroscopy I	3	60		
	CP-5-CHM-106	Practical	5	100		

CONTENTS

SEM-I	CT-3-CHM-101	Inorganic Chemistry	Chemical Bonding, Acid-Base-Redox Chemistry, Structure of simple solids, Chemistry of transition metals
	CT-3-CHM-102	Organic Chemistry	Structure, Bonding and Reactivity, Reaction Mechanism, Stereo-Chemistry, Disconnection Approach
	CT-3-CHM-103	Physical Chemistry	Equilibrium and Thermodynamics, Non-equilibrium Thermodynamics, Statistical Thermodynamics
	CT-3-CHM-104	Quantum Chemistry I	Basic principles of quantum mechanics, particle in a box problems, operator algebra, Simple Harmonic Oscillator, treatment of H-atom, Approximate methods, Antisymmetry Principle.
	CT-3-CHM-105	Spectroscopy I	Rotational (microwave) spectroscopy, Raman Spectroscopy, vibrational spectroscopy, photoelectron Spectroscopy, Electronic Spectroscopy and their applications
	CP-5-CHM-106	Practical	Inorganic Lab, Organic Lab & Physical Lab

SEM-I	CT-3-CHM-101	Inorganic Chemistry	Chemical Bonding, Acid-Base-Redox Chemistry, Structure of simple solids, Chemistry of transition metals

Unit-I Chemical Bonding & Electronegativity Marks 15

LCAO-MO methods in homo and heteronuclear diatomic molecules (O_2, N_2, CO, NO). MO description of tri and tetraatomic molecules (CO_2, NO_2, NO_2^+, CO_3^{-2}, O_3 and NO_3^-.

Metallic bonding: Band theory of Solids – conductor, semiconductor and insulators. Superconducting oxides. Spinel and Perovskite structures.

VSEPR Theory: Structure of molecules containing lone pair(s) of electrons, structure and hybridization, Bent's rule, Bent bond, Non-bonded repulsion and structure.
Mulliken-Jaffe electronegativity scale, spectroscopic electronegaitvity, Absolute and group electronegativity. Chemical hardness, Application of electronegativity.

Unit-II : Acid Base and Redox Chemistry Marks 15

Acid-Base concepts, Measure of Acid-Base Strengths, Acid-Base in water. Non-aqueous solvent, aprotic solvent and superacids. Hard and Soft Acids and Bases, application of SHAB principle.
Half cell reaction, reduction potential, application of reduction potential data, electrochemical series; brief idea of corrosion and its prevention; Nernst equation. Latimer and Frost diagram, disproportionation reaction; cyclic voltametry.

Unit-III : Structure of simple solids Marks15

Packing of spheres – hexagonal and cubic close packing, tetrahedral and octahedral holes in close-packed structures- metals and alloys, solid solutions. The ionic model for the description of bonding in ionic solids. Characteristic structures of ionic solids- the NaCl and CsCl types, the sphalerite and wurtzite types of ZnS, the NiAs structure type, the perovskite and spinel structure types of mixed-metal oxides- importance ionic radii and the radius ratios in determining structure type among ionic solids. Lattice energy considerations, thermal stability and solubility of inorganic solids.

Unit IV: Properties of transition metal complexes: Marks 15

Transition metals and periodic properties. Transition metal donor-acceptor compounds, Coordination number and geometries, 18-electron rule, Stability of metal complexes, common ligands and complexes, Stereochemically non-rigid systems.
Metal ligand bonding: Ionic surrounding: Crystal Field Theory; Covalent surrounding: Transition metal MO and ligand field Theory, Transition metal complexes with π-bonding ligands.
Molecular orbital model, General view of ML_6 and ML_4 structures: ML_6 (O_h), ML_4 (D_{4h}) and ML_4 (T_d), The Angular overlap model (Qualitative) Jahn-Teller Distortion from O_h geometry.

SEM-I	CT-3-CHM-102	Organic Chemistry	Structure, Bonding and Reactivity, Reaction Mechanism, Stereo-Chemistry, Disconnection Approach

Principles of Organic Chemistry

Unit I Marks 15

Structure, bonding and reactivity of organic compounds : Aromaticity, antiaromacity and homoaromaticity, metallocenes, tropolones and azulenes. Bonds weaker than covalent bond – charge transfer complexes, inclusion complexes and crown ethers. Cryptand, rotaxanes, Fullerenes, Graphenes. Phase transfer catalyst.

Hammet equation, Taft equation. Influence of reaction medium on rates.HSAB concepts and their applications.

Unit II Marks 15

Organic reaction mechanism – Transition state vs. Reaction intermediate, Energy profile of multistep reaction, Significance of rate limiting step in multistep reactions, Catalysed and uncatalysed reactions, Kinetic vs. Thermodynamic control, Kinetic and non-kinetic methods of studying organic reaction mechanism; Isotope labeling studies and kinetic isotope effects, Cross-over experiment. Reactivity - selectivity principle : Chemoselectivity, regioselectivity, stereoselectivity and stereospecificity in substitution, elimination and addition reactions. Neighbouring group effects.

Unit III Marks 15

Stereochemistry– Molecular symmetry, asymmetry and dissymmetry; Classification of organic molecules into different point groups, Concept of prostereoisomerism and prochirality – Homotopic and heterotopic ligands and faces; Optical purity and enantiomeric excess; Chirality in molecules devoid of chiral centers - allenes, spirans and biphenyls.

Classification of stereoselective synthesis: diastereoselective and enantioselective reactions; Stereo-differentiating approach, Nucleophilic addition to aldehydes and acyclic ketones: Cram and Felkin – Ahn model. Enantioselective synthesis – Use of chiral reagent, chiral catalyst and chiral auxillary.

Unit IV Marks 15

Disconnection approach in organic synthesis: Retrosynthesis of Alcohols (Grignard approaches and hydride transfer approaches) and Carbonyl compounds. Acceptor and donor synthons, Use of umpolung, One group and two group C-X disconnections. One group and two group C-C disconnections. Retrosynthsis of 1,2-, 1,3-, 1,4-, 1,5- and 1,6- difunctional (O,O and N,O in a difunctional relation) compounds.

Use of protecting groups in organic synthesis : protection and deprotection of hydroxyl, dihydroxy, carbonyl, carboxyl and amino groups.

Sem I	CT-3-CHM-103	Physical Chemistry	Equilibrium and Thermodynamics, Non-equilibrium Thermodynamics, Statistical Thermodynamics.

Equilibrium and Thermodynamics: **Marks 20**

Concept of fugacity and it determination. Ideal solution and non ideal solutions, Activity and activity coefficient, Determination of activity coefficient, excess function for non-ideal solutions. Partial molar quantities: chemical potential, Determination of partial molar volume, Thermodynamics of mixing. Third law of thermodynamics, its experimental verification, determination of absolute entropy.

Non equilibrium thermodynamics: **Marks 20**

Difference between equilibrium and non-equilibrium thermodynamics, Criteria of non-equilibrium thermodynamics; uncompensated heat and its relation to other thermodynamic functions, Fluxes and forces- relation between these two quantities, Entropy production in heat transfer, mass transfer in flow of current, in mixing of gases, and in chemical reaction; phenomenological relation: Onsagar relation, microscopic reversibility and Onsager reciprocity. Coupled reaction. Thermoelectric effects: Seebeck, Peltier and Thompson effect

Statistical thermodynamics: **Marks 20**

Part1: Maxwell-Boltzmann distribution law, Bose-Einstein and Fermi-Dirac distribution law. Boltzmann relation between entropy and probability. Partition functions and thermodynamic functions. Thermodynamic functions of a monatomic gas, Sackur – Tetrode equation. Evaluation of translational partition function using particle in a box model for ideal monatomic gas.

Part2: Rotational and vibrational entropy of gases, Residual entropy, Free energy and partition functions. General expression for partition function and equilibrium constant. Energy and heat capacity of gasses. Einstein and Debye’s theory of heat capacity of solids.

Part3: Calculation of energy and Entropy, heat capacity of polyatomic molecules CO_2, SO_2 etc. Numerical calculations of thermodynamics functions for diatomic and polyatomic molecules.

Sem. I	CT-3-CHM-104	Physical Chemistry	Quantum Chemistry I

1. Basic principles of quantum mechanics: Postulates, Hermitian operators, commutation relation. Free particle and particle in a box (One and three dimensional), degeneracy. Postulates; operator algebra; exactly- solvable systems,) Eigenvalues and eigenfunctions of quantum mechanical operators, their physical significance. Schródinger's wave equation. Orthogonal functions – Schmidt's orthogonalisation technique. Basic ideas about the theory of angular momenta – spin and orbital angular momenta, conservation of angular momenta. General angular momentum operators J_x, J_y, J_z step-up and step-down operators, Eigenvalues of J^2 and J_z operators. Coupling of orbital and spin angular momenta – theoretical basis of the L-S and j-j coupling schemes. **Marks 20**

2. Simple Harmonic Oscillator-Schrodinger equation and its solution. Two-particle rigid rotor- rotational energy levels of diatomic molecules, particle in a ring, quantum mechanical tunneling. **Marks 12**
3. Hydrogen atom- Schrodinger equation, separation of relative coordinates, radial solution, probability and radial distribution function, angular solution, representation of orbitals, shapes of atomic orbitals, orbital and spin angular momentum. **Marks 12**
4. Approximate methods: Variation theorem, Linear variation functions. Time independent Perturbation theory for non-degenerate systems (up to second order in energy); application to the helium atom. Hellmann-Feynmann theorem. **Marks 12**
5. Antisymmetry Principle, Slater determinant, Term symbol, spectroscopic states.

Marks 4

Sem.- I	CT-3-CHM-105	Spectroscopy I	Rotational (microwave) spectroscopy, Raman Spectroscopy, vibrational spectroscopy, photoelectron Spectroscopy, Electronic Spectroscopy and their applications

Unit I:

Introduction: Electromagnetic spectrum, interaction of electromagnetic radiation with molecular systems; Spectroscopic transition- absorption, emission, reflection, polarization and scattering processes; Natural line width and broadening- intensity of spectral transitions, selection rules; sampling techniques in different branches of spectroscopy.

Marks 5

Unit II: **Marks 10**

Rotational (microwave) spectroscopy: Classification of molecules according to their moments of inertia, rotational energy levels of HCl, Selection rule for Microwave spectra, intensity, effect of isotopic substitution in Microwave spectra. Stark effect, spectra of symmetric top and asymmetric top type molecules

Unit III: **Marks 8**

Quantum theory of Raman Effect, Selection rules, mutual exclusion principle, vibration-rotation Raman spectra. Intensity of Raman lines.

Unit IV: **Marks 12**

Fundamental vibrational frequencies, Selection rules and vibrational energy for harmonic and anharmonic oscillators, vibration rotational spectra of diatomic molecules, Fundamental, overtone and combination bands, P, Q and R branches, hot bands, group frequencies, normal modes of vibrations, Finger print region, effects of hydrogen bonding on band frequency-problems..

Unit V: **Marks 8**

Introduction to Photoelectron Spectroscopy: Auger electron spectroscopy. Chemical information from ESCA

Unit VI: **Marks 12**

Chemical shift, factors affecting chemical shift, spin- spin interaction, Coupling constant and Factors affecting, relaxation processes, NOE, Nuclear magnetic double resonance, shift resonance, spin tickling; Proton and ^{13}C NMR spectroscopy of simple organic molecules, living systems – MRI, : Two dimensional NMR, NOESY, DEPT, INEPT terminology, Instrumentation, FT NMR.

Unit VII: **Marks 10**

Electronic spectroscopy: Electronic transitions and selection rules, Frank Condon principle and electronic spectra of polyatomic molecules, Luminescence: Fluorescence and phosphorescence, solvent effects, absorption and intensity shifts, Calculation of absorption maxima by Woodward-Fieser Rules.

Sem I	CP-5-CHM-106	Practical	Inorganic Lab, Organic Lab & Physical Lab

Group I: Inorganic Lab **Marks: 20**

Preparation and characterization (viz. conductivity measurement, IR, UV-Vis) of the following complexes:

1. Sodium ferrioxalate, $Na_3 [Fe (C_2O_4)_3] 9H_2O$
2. Potassium chromioxalate, $K_3[Cr(C_2O_4)_3]$
3. Tris-(thiourea) copper (I) sulphate, $[Cu(tu)_3]_2SO_4.2H_2O$
4. Tetraamine Cu (II)sulphate, $[Cu(NH_3)_4]SO_4.H_2O$
5. Hexa-amine Ni (II) chloride $[Ni(NH_3)_6]Cl_2$

Group II: Organic Lab **Marks: 20**

Systematic qualitative analysis of organic compounds – Separation and identification of organic compounds from two component mixtures, each having more than one functional group.

Group III: Physical Lab **Marks: 20**

1. To determine the rate constant of hydrolysis of methyl acetate catalyzed by an acid and also the energy of activation.
2. To determine the velocity constant of hydrolysis of ethyl acetate by NaOH.
3. Determine the rate constant of inversion of cane sugar by analytical method.
4. Study the kinetics of the reaction between iodine and acetone in acidic medium by half-life period method and determine the order with respect to iodine and acetone.
5. Determine the molar mass of a polymer by viscometric method.
6. Study the complex formation between Cu^{2+} ion and ammonia by distribution method and find the composition of the complex.
7. To determine the radius of a molecule (glycerol) by viscosity measurements.

IV. Viva-voce Marks **10**

V. Internal Assessment Marks 30 **(3 × 10 = 30)**