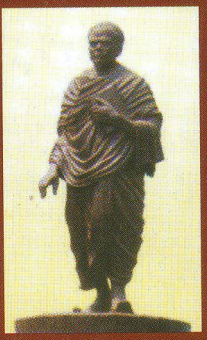
DIRECTORATE OF DISTANCE EDUCATION



SYLLABUS

M.Sc. Course in Chemistry

VIDYASAGAR UNIVERSITY
MIDNAPORE - 721102

VIDYASAGAR UNIVERSITY

Department of Chemistry & Chemical Technology

Syllabus

(M.Sc. Course in Chemistry)

Distribution of Papers and marks

M.Sc. Part-I

Paper	Marks	
	Theoretical	**Practical**
I. (Physical Chemistry)	75	50
II. (Organic Chemistry)	75	50
III (Inorganic Chemistry)	75	50
IV (Industrial Chemistry	75	50*
Total	**300**	**200**

* Industrial = 20, Computer = 20, Industry visit = 10

M.Sc. Part-II (Special #) # Physical/Organic/Inorganic

Theoretical Papers	Marks	Practical Papers	Marks
V	75	Special Practical	150
VI	75		
VII	75	Professional/Project	50
Professional Paper)	♦75		
Total	**300**		**200**

Polymer Science for Physical & Organic Special, Environmental Chemistry for organic Special.

M.Sc. Part-I

Paper-I FM-75

Physical Chemistry (General)

Unit

01. Quantum Mechanics: (15-20 lectures)

The wave-particle duality and the development of Schrödinger equation, interpretation of ψ, postulates of quantum mechanics with necessary explanations, formulation of quantum mechanical operators, angular momentum operators (in cartesian and polar co-ordinates), step-up and step-down operators, commutation relations; the Gedanken experiment to derive an expression for the uncertainty principle; free particle, particle in a box, particle in a ring, particle in a sphere, free electron molecular orbital (FEMO) model; one dimensional harmonic oscillator, rigid rotator (in three dimensions), potential barrier, tunneling, hydrogen atom, concept and shape of orbital, space and spin quantisation; the Aufbau principle and the many electron atom, vector atom model and the spectroscopic states; hydrogen molecular ion and the concept of molecular orbital, hydrogen molecule; homo-and hetero-nuclear diatoms, importance of overlap, hybridization.

Elementary idea of variation and perturbation theorems with some simple applications.

02. Classical and Statistical Thermodynamics, Transport Phenomenon: (15-20 lectures)

Maxwell's relations, thermodynamic equation of state; partial molar quantities, thermodynamics of mixing, activity and fugacity. Nernst Heat theorem, third law of thermodynamics. Thermodynamic probability and entropy. Maxwell-Boltzman, Bose-Einstein and Fermi-Dirac statistics. Partition functions of diatoms (translational, rotational, vibrational and electronic). Young-Laplace equation, Kelvin equation, surface (interface) thermodynamics. Adsorption, adsorption isotherms (Langmuir and BET

with derivation). Surfactants, micelles, reverse micelles and emulsions and their applications.

Distribution of molecular velocities, principle of equipartition of energy, collision frequency, thermal conductivity, general diffusion expression and Fick's laws general features of transport of matter (diffusion), thermal energy (thermal conductivity) and momentum (viscosity).

03 Electrochemistry (15-20 lectures)

Mean activity co-efficient of electrolytic solutions, Debye-Huckel theory, ion association, precise determination of dissociation constants of weak electrolytes – e.m.f and conductometric methods, the Onsager conductance equation, effect of high electric field and high frequency on ion conductance; polarography, overvoltage, surface tension of electrolytic solutions, polyelectrolytes. Basic principle of cyclic voltametry and coulometry.

04 Chemical Kinetics (15-20 lectures)

Principle of detailed balancing (simple idea only), opposing and consecutive reactions, static, flow and relaxation methods of measurement of reaction rates, flash photolysis. Kinetics of fast reaction, collision theory of reaction rates (detailed), preliminary idea of transition state theory.

Homogeneous and heterogeneous catalysis, autocatalysis, oscillatory reactions (general introductions only), redox reactions, preliminary idea of inner sphere and outer sphere reactions of transition metals.

05 Molecular Structure and Molecular Spectroscopy (15-20 lectures)

Dielectric polarisation, Debye-Langev in equation, dipole moment – determination and applications, intermolecular forces and their contribution to intermolecular potential. General features of molecular spectra, quantum mechanical rigid rotator, pure rotational spectra of linear molecules, non-rigid rotator, expression for centrifugal distortion constant; quantum mechanical harmonic oscillator, vibrational spectra of diatoms,

anharmonicity and molecular dissociation, hot band and overtones, zero point energy and uncertainty; rotational and vibrational Raman spectra – general features and applications, principle of mutual exclusion.

Vibrational structure of electronic spectra. Frank-Condon principle.

Photoionisation of atoms and molecules, electron energy analyzer and photoelectron spectra, molecular orbitals and photoelectron spectra.

Books Recommended :

1. Physical Chemistry : Berry, Rice and Ross.
2. Physical Chemistry : Moore.
3. Physical Chemistry : Atkins
4. Physical Chemistry : Levine
5. Chemical Kinetics : Laidler
6. Kinetics and Mechanism : Frost and Pearson
7. Heat and Thermodynamics : Zemansky and Dittman
8. A Treatise on Heat : Saha and Srivastava
9. Quantum Chemistry : Eyring. Water and Kimbal
10. Quantum Chemistry : Pilar
11. Quantum Chemistry : Levine
12. Electrochemistry : Glasstone
13. Electrochemistry : Bockris and Reddy
14. Molecular Spectroscopy : Banwell
15. Molecular Spectroscopy : Barrow
16. Molecular Spectroscopy : Grabeal
17. Molecular Spectroscopy : Chang.

M.Sc. part-I

(Physical General) Practical

Unit

01 **List of Experiments :**

[1] Determination of the exact concentration of HCI solution of N/10 order by NaOH Conducometorically.

[2] Determination of the exact concentration of oxalic acid solution of N/10 order by NaOH Conducometrically.

[3] Determination of the exact concentration of KCI solution of N/10 order by $AgNO_3$, Conductmetrically.

[4] Determination of exact concentration of KCI solution of N/10 order by $AgNO_3$, Potentiometrically.

[5] Study of the Kinetics of Inversion of Cane sugar by polarimetry.

[6] Study of Kinetics of Iodination of Acetone in presence of Acid. Hence find out the order with respect to iodine or acetone.

[7] Determination of Partition Co-efficient of Benzoic acid between Water & Benzene. Hence show that benzoic acid dimerizes in benzene layer.

[8] Determination of Critical Solution Temperature of Phenol-Water system.

[9] Determination of Solubility Product of PbI_2 and verification of Debye-Huckel limiting law.

[10] Find the absorption maximum of an aqueous $KMnO_4$ solution and verify Beer's Law.

[11] Determination of E of quinhydrone electrode.

[12] Determination of exact concentration of HCI and oxalic acid in their mixture conductometrically.

[13] Determination of composition of copper(II)-ammonia complex analytically.

[14] Determination of dissociation constant of weak acid (acetic acid, benzoic acid) by pH measurement.

At least ten (10) experiments are to be performed by a student of M.Sc. part-I (Physical general) during the laboratory session.

Practical Examination of M.Sc. Part-I Physical general :

Unit 01 :

Physical Chemistry Experiments [Two days (Six hours each day) examination]

Total Marks : 30 (thirty only).

Unit 02 :

Internal Assessment.

Total Marks : 10 (ten only).

Unit 03 :

Viva-voce and Laboratory Note Book (during examination)

Total Marks : 10 (ten only)

M.Sc. Part-I, PAPER – II

ORGANIC CHEMISTRY (GENERAL)

(Every unit consists of 15-20 lectures, Full Marks =75)

Unit

01 **Structure and Reactivity of Organic Molecules :**

Advanced reaction mechanisms, delocalized systems-cyclic and acyclic (M.O.approach). Concept of aromaticity, antiaromaticity and homoaromaticity. Introductory course on pericyclic reactions – electrocyclic reactions, sigmatotropic rearrangements, cycloadditions, Rationalization on the basis of Frontier Orbital Theory, Hammett Equation and applications. Nonclassical carbocations . Advanced treatment of topics of reaction mechanisms included in B.Sc (Hons) syllabus.

02 **Stereochemistry and Conformational Analysis**

Symmetry and molecular chidrality. Stereochemical nomenclature for acyclic and cyclic molecules. Conformation in acyclic and cyclic systems – energy barrier to rotation, potential energy profiles. Conformation and physical properties of 6-membered rings and reactivity in acyclics. Stereochemistry of trivalent carbon.

Prostereoisomerism, Asymmetric synthesis – addition of achiral reagents to chiral ketones and aldehydes. Models for stereochemical control, Cram, Karabatros and Fehlkin models, sterospecific and stereoselective reactions. Molecular rearrangements – generalized treatment of stereochemical features.

03 **Heterocyclic Chemistry and Spectroscopy :**

Monocyclic and bicyclic heterocycles having one or two heteroatoms principles of NMR spectroscopy (elementary ideas). Application of UV IR and NMR in structure elucidation of organic molecules.

04 **Natural Products ; Bioactive Molecules :**

Terpenoids : Isoprene rules, acyclic monoterpenoids such as citral, geraniol, neral, linalool, monocyclic, terpenoids menthol. aterpineol. Alkaloids : phenylethylamine series, coniine, nicotine. Synthesis and reactions of heterocycles : generalized approach.

Isolation, structure elucidation, sydnthesis and biogenesis of representative examples of Proteins and Peptides (elementary ideas), Nucleosides and Nucleotides (elementary ideas).

05 **Synthetic Methodology and Reagents :**

Retrosynthetic analysis, disconnection approach, functional group intercoversions; examples to illustrate disconnection approach to organic synthesis.

Organophosphorous and organosulfer reagents, organoboranes, organosilanes, organostannanes, metal hydrides, Birch reduction, hydroxylation reagents, uses of peracids. Woodward and Prevost hydroxylation. Mitsunobu reaction. Sharpless epoxidation. Bayer-Villiger reaction, Chichibabin reaction and newer methods in organic synthesis. Phase transfer catalysis, reactions on solid supports, Merrifield resin, solid-phase synthesis, template synthesis.

References :

1. Advances in Organic Chemistry, Part A and B, F.A. Carey and R.J. Sundberg.
2. Advances in Organic Chemistry, Jerry March, McGraw Hill.
3. Organic Chemistry. R.T.Morrison and R.W. Boyd. Wiley Eastern.
4. Organic Chemistry. S.H. Pine. McGraw Hill.
5. Fundamentals in Organic Chemistry. T.W.G.Solomons, John Wiley.

M.Sc. Part – I

(Organic Chemistry Practical)

(Two days examination – 6 hours per day, Full Marks = 50)

Unit

01 **(a) Qualitative Analysis of Solid Organic Compounds leading to**

(i) Detection of elements (N.Cl.Br.I.S) : Solubility tests.

(ii) Systematic Analysis to detect the functional groups : alcoholic/ phenolic OII, Carboxylic, alehydes, ketone, ester, nitro, amino, amido, N-substituted amino, imido groups, unsaturation (C=C) aromatic hydrocarbons and halogenated derivatives.

(iii) Preparation of Crystalline derivatives/suitable derivatives to identify the compound.

Students will have to analyse atleast 6 (six) samples including solid compounds during their course work.

Each candidate during the examination shall be assigned one solid sample for analysis during the examination. (20)

(b) Preparation of pure organic compound by single-step or two step procedure. Submission of crystallised produced.

02 **Sessional Work** (15)

To be awarded by the class teacher on the basis performance of the students during the course work. (5)

03 **Viva Voce**

To be jointly conducted by the external and internal examiners during the examination. (10)

M.Sc. Part – I, PAPER – III

INORGANIC CHEMISTRY (GENERAL)

(Every unit consists of 15 – 20 lectures, Full Marks = 75)

Unit

01. Symmetry and Group Theory

Groups and their properties : The concept of groups, Group Multiplication tables and rearrangement theorem, subgroups and classes.

Symmetry elements and operations of molecules and crystal systems. Point groups : molecular and crystallographic, Matrix representation of symmetry operators.

Representation of point groups : Matrix representation of point groups, reducible and irreducible representations, the great Orthogonality theorem (without deriviation) and its corrolaries, construction of character tables in simple cases (C D), reduction of a reducible representation, direct product and its decomposition.

Models of MO and VB theories – application to H H qualitative M.O. theory – energy levels of homo – and hetero – nuclear diatomic molecules of second period elements, equivalence of MO and VB theories, electronic structure of solids – band theory.

02. COORDINATION CHEMISTRY

Crystal Field theory, Adjusted Crystal Field Theory, Distortions (tetragonal and trigonal), crystal field stabilization energy, thermodynamic aspects of crystal field splitting (Variation of ionic radii, lattice-energy, hydration energy), Kinetic aspects of crystal field splitting (labile and inert complexes). Qualitative MO treatment : the electronic structure of the MI (octahedral) and ML_4 (tetrahedral) complexes on the basis of simple symmetry and overlap principles, energy level diagrams. - d transitions in weak field cases, Orgel diagram and electronic spectra of transition metal complexes (d_1 - d_9) effort of substitution, spectro chemical series,

charge transfer spectra. Magnetic properties of free ions and metal complexes – a qualitative approach.

Complex formation in solution : stability constants (overall and stepwise), Irving – Williams order, methods for the determination of complex composition (Job's, mole ratio and slope ratio methods), Bjerrum's half integer method for the decom-position of stability constants, chelate effect and macrocyclic effect.

03. Chemistry of d-block elements

Chemistry of 3d, 4d and 5d transition metals i.e. Ti –Hf, v-Ta, Cr –W, Mn – Re and platinum metals with reference to

(i) Aqueous chemistry, oxidation states, co-ordination number and complexes, redox behaviour.

(ii) Iso-and hetero – polyacids and salts of Mo.W.

(iii) Di nit gen and di oxygen complexes.

(iv) Intramolecular charge transfer : Creutz – Taube ion.

(v) Binary carbonyl complexes : structures and bonding.

(vi) Property, structure and bonding ion, molybdenum blue, tungsten blue, tungsten bronze, ruthenium red, Creiutz – Taube complex, Nb, Ta halide clusters.

Introduction to organometallic chemistry : definition and classification (on basis of ligand type), examples of carbene and carbyne complexes. hapticity, structure and bonding in η^2ethylenic and η^3allylic complexes, fluxional molecules.

Essential elements in Biology (major and trace), beneficial and toxic elements, role of metal ions in biology – metalloproteins and metalloenzymes : transport and storage proteins (Ferritin and Transferrin), dioxygen carrier and storage proteins (haemoglobin and myoglobin), electron transfer proteins : ferredoxin, rubredoxin etc. nitrogen fixation.

04 **Chemistry of main group and inner transition elements**

Relative effects on chemical properties, noble gas clath rate compounds, structure and bonding in boranes and carbenes, silicates and silicone, inorganic chain, ring and compounds : B N.P. – N.P – O and S – N compounds, interhalogen, halogen oxides and oxygen fluorides.

E.S R spectroscopy : general background, representation of ESR spectrum, 'g'-value, spectra of simple organic free radicals – hyperfine coupling, prediction of expected number of lines and intensities, spectra of transition metal complexes-metal hyperfine, anisotropic spectra, zero – field splitting, applications (only examples).

Reaction mechanism : preliminary ideas on different types of mechanisms (A.D.I la. I etc.) of substitution reactions for inorganic complexes, examples, an idea on trans effect.

05 **Analytical Techniques and Methods**

Spectroscopic methods : spectrophotometry – basis principles, applications (photometric titration, estimation). Atomic Absorpdtion spectroscopy – basic principle, concentration and absorbance, caibration, interferences, an idea on instrumental set up, applications (detection/ estimation of metallic elements in ores and alloys). Fluororescence spectroscopy – basic principles and applications. Flame photometry – basic principles and application. Electro analytical methods : polarography – Cyclic voltametry and coulometry and some applications.

M.Sc. Part –I

(Inorganic Chemistry Practical)

(Two days examination - 6 hours per day, Full Marks = 50)

1) Qualitative Analysis : Detection of six radicals (including two from rare metals) from a mixture.

2) Qualitative Analysis : Mixture : Ni $^{2}/Mn^{2}$: Cr $^{3}/Mn^{2}$
Alloys : Gun metal (Cu/Sn)
Ore : Pyrolusite

3) Preparation and composition study : (at least one)
Potassium trioxalato ferrate (III)
Potassium trioxalato chromate (III)
Ammonium tetra nitro nickelate

M.Sc. Part-I, Paper IV

Chemical Technology

(Every unit consists of 15 – 20 lectures, Full Marks = 75)

Unit

01 **Fluid dynamics**

Fundamental principles of fluid mechanics, Newtonian and Non-newtonian fluids. Streamline and turbulent flow. Pressure drop calculation for flow through pipes and channels, Hagen Paisonallies equation. Bernonli's equation. Flow measuring instruments, Manometers, Filtration, different filters.

02 **Heat transfer**

Heat transfer by conduction. Steady and unsteady state of heat transfer, Heat transfer by convection, Natural and forced convection. Heat transfer by radiation. Heat emmission and absorption by black, natural and grey bodies.

03 **Unit Process and stocihiometry**

Unit processes in organic synthesis including nitration, hydrogenation, oxidation, sulfonation, esterification and polymerisation. Industrial stoichiometry, material and energy balance, solution of problem. Chemical reactions, isothermal, adiabatic and non-isothermal and non-adiabatic, Design equation. Heat and mass transfer effect on catalytic reaction.

04 **Mass transfer operation and Ore Processing/Beneficiation**

Mass transfer : Principle of diffusion and mass transfer, mechanism of mass transfer, simultaneous heat and mass transfer. Ficks' law, application.

Ore Processing/Beneficiation : Definition of an ore, Types of ores, operating steps involved in ore processing/dressing/benefication: coominution, sizing and screening, concentration and fitter processing. Different process of concentration of ore minerals. Beneficiation of Pb-Zn-Cu ore. Iron ore, Zn ore etc. Beach sands and graphite, leaching as a means of ore processing.

05 **Fuel and refractories**

Solid, liquid and gaseous fuels, coal origin, proximate analysis and ultimate analysis, combustion. Petroleum and refineries, products, synthetic liquid fuels. Bergious process, Fischer Tropsch process.

Refractory materials.

Nomenclature, classification acidic, basic and neutral refractories, production, important properties and uses.

M.Sc. Part – I

Practical

INDUSTRIAL CHEMISTRY PRACTICAL

Marks = [20]

01. (a) Quantitative Analysis Experiments [05]

(1) Analysis of Portland cement

(2) Analysis of Soda ash/coal ash/fly ash

(3) Analysis of basic slag

(4) Analysis of water (hardness)

02. (b) Demonstration type experiments to be performed in groups. [05]

Study and use of orifice meter, venture meter, pitot tube Rayleigh

(1) Distillation and other skills. Bomb calorimeter, Junckers calorimeter.

(2) Determination of surface area by air permeability method.

(3) Determination of viscosity of liquid by falling sphere method

(4) Determination of viscosity of fuel oil (Red woods viscometer)

(5) Proximate analysis of coal samples

(6) Orsat analysis

(7) Determination of flash point of a fuel oil

(8) Determination of diffusion coefficient of liquid vapour through air by

(09) Stefens method

(10) Distillation of binary liquid mixture to verify Reileigh equation.

03. Sessional [05]

04. Viva-voce [05]

Computer Science Marks = 20

Theory :

History of development of computer mainframes, minis, micros and Supercomputer. Computer hardware, CPU and other peripheral devices (input/output and auxiliary storage devices), introduction to software and programming languages, Machine language, assembly language and higher level languages. Details of Fortran 77 – and its application in solving simple problems like solution of quadratic equation, summation of nhotwral numbers, finding Harvard deviation, sorting of numbers, 1st order reaction, software packages : d BASE LOTUS, WORD STAR, WINDOW.

Practical :

Application of Fortran – 77 of the problem mentioned in the theory in PCXT – minicomputer, Word Star.

Industry visit Marks = 10

M.SC. Part – II

Paper V, FM – 75

Physical Chemistry Special

Unit

01 Mathematical Methods and Quantum Mechanics – I **(15-20 lectures)**

Mathematic methods : Polynomial fitting by method of finite difference, Newton's first and second difference formula, numerical methods of integration, accumulation of error due to arithmetical operations, iterative methods of solutions of polynomials and simultaneous equations.

Probability and flux density, continuity equation. Superposition principles and their expansion theorem, matrix representation of operators, spin operator and Pauli spin matrices, many electron atom and construction of wave function for spectroscopic states; projection operator, their properties and applications. Density matrix.

Stern-Garlach experiment and double Stern-Garlach experiment, simultaneous measurability and commutability, uncertainty principle; Heisenberg's equation of motion, constants of motion, virial theorem, parity, time reversal symmetry.

02. Quantum Mechanics – II **(15 – 20 lectures)**

Variation principle, stationary state perturbation theory for degenerate and non-degenerate states, time dependent perturbation theory.

Applications of variation and perturbation theories : expression for polarizability, helium atom in its ground state, Stark effect, Zeeman effect.

Approximation methods : HMO and EHMO methods and their applications.

03 Quantum Mechanics – III **(15 – 20 lectures)**

Independent particle model, Hartree SCF method and Hartree-Fock theory for closed and open shell, Roothan-Hartree-Fock theory and their application. Brillouin's theorem and Koopman's theorem, limitations of independent particle model and electron correlation.

Elementary idea of ab initio and semiempirical methods in computational chemistry and their application to structure, reactivity and reaction path calculations.

04. Group Theory **(15 – 20 lectures)**

Symmetry properties, symmetry transformations, symmetry groups and sub groups. Finite and continuous groups. Matrix representations of point group and translational groups, reducible and irreducible representations, characters, projection operator, direct product representation, vanishing integrals and their applications.

The Great Orthogonality theorem (statement only and applications), character tables. Application of group theory to orbital sydmmetry, molecular spectra, ligand field transitions and vibration of polyatomic molecules.

05 Solid State Chemistry **(15 – 20 lectures)**

Unit cell, reciprocal lattice, Bragg's law, Laue's diffraction, geometrical structure factor, Fourier synthesis, Patterson function, lattice dynamics, normal modes, phonons, thermal conductivity, electrical conductivity, Hall effect and quantum Hall effect.

Free electron theory, thermo ionic emission and plasma frequency; wave function in a periodic lattice, Bloch's function; hole and charge carriers, band structure of metals, conductors, semiconductors, super conductors and insulators.

Magnetic properties of solids: para-, ferro-, antiferro-and diamagnetism, typical examples.

Theory of photoconductions, excitons; photoconducting and photovoltaic effects.

Paper VI FM -75
Physical Chemistry Special

Unit

01 Statistical Mechanics (15 – 20 lectures)

Concept ensemble and phase space, ergodic hypothesis; Microcanonical ensemble: partition function, temperature; Canonical ensemble : distribution, probability and partition function. Partition function and different thermodynamic state functions. Gibbs paradox. Molecular partition functions : translational, rotational, vibrational, electronic, and nuclear. Applications : Principle of equipartition of energy, chemical equilibrium, Saha ionization formula.

System of interacting particles, imperfect gas.

Grand canonical ensemble : Nature of quantum particles, Bose-Einstein and Fermi-Dirac statistics, specific heat of electron gas. Bose-Einstein condensation. Quantum statistics, density matrix.

02 Non-equilibrium Thermodynamics, Mossbauer Spectros copy (15 – 20 lectures)

Entropy production in irreversible processes, Onsager reciprocal relations, principle of microscopic reversibility, thermonuclear pressure difference and thermonuclear effect, cyclic and oscillatory reactions, non-linear region, higher order symmetries.

Mossbauer Spectroscopy : Principle, experimental setup, center shift, quadrupole interaction, magnetic interaction, Mossbauer spectra of iron compounds. Applications : study of spin, oxidation states, bonding and spin transitions.

03 Advanced Electrochemistry (15 – 20 lectures)

Modifications and extensions of the Debye-Huckel theory, surface tension of electrolytic solutions, theories of solvent interaction, non-stationary processes in electrolytic solutions, hydrogen overvoltage, thermodynamics of ideally polarized electrodes, metal-electrolyte and semiconductor-electrolyte interfaces. Fuel cells.

04 Chemical Kinetics (15 – 20 lectures)

Transition state theory, potential energy surface and contour. Reaction path; valley and saddle point. Computation of potential energy — elementary idea of ab initio method; empirical methods: London-Eyring-Polyani-Sato (L.E.P.S), bond-energy-bond-order (BEBO) method. Saddle point – activation energy.

Statistical formulation of chemical kinetics, equilibrium formulation, derivation of expression for specific reaction rate. Thermodynamics of reaction rates, expression for rate constant after. Eyring equation, entropy of activation.

Reactions in molecular beams; reactions and shock waves. Theory of absolute reaction rates and its applications in viscosity and diffusion.

05 Macromolecules and Biopolymers (15 – 20 lectures)

Molecular weight of polymers, molecular weight determination by light scattering, sedimentation, diffusion, osmotic pressure, and viscosity measurements. Thermodynamics of polymer solutions, heat and free energy of mixing. Equilibrium properties of polymer solutions, viscoelastic properties of high polymers. Kinetics of macromolecule formation.

Structure of biomolecules : (1) Proteins-building blocks,peptide bonds, primary, secondary, tertiary, quaternary structures, phi-psi map (2)_ Nucleic acids – A, B, Z conformations, t-RNA conformation. Carbohydrates and lipids-biomembranes. Techniques to study biomolecules : CD, ORD, fluorescence, IR and Raman spectroscopy (simple applications).

Methods for determination of molecular weight of biopolymers : (a) SDS-PAGE (for proteins), (b) agarose gel method (for nucleic acids). Polymer conformation statistics of linear polymers.

Paper VII FM - 75
Physical Chemistry Special

Unit

01 Molecular Spectroscopy (15 – 20 lectures)

Interaction of matter with radiation. Fermi's Golden rule, Born-Oppenheimer approximation. Selection rule for pure rotational spectra, vibrational spectra, rotational and vibrational Raman effect (Quantum mechanical formulations).

Rotational spectra of polyatomics : Spherical top, symmetric top, and asymmetric top molecules. Internal rotation, nuclear spin and rotational energy level. Stark effect, Coriolis coupling. Vibration of polyatomic molecules : Normal modes and their symmetry, overtones, combination bands and hot bands. Introduction to normal co-ordinate analysis, localised group vibrations, non-genuine vibrations. Torsional oscillations. Fermi resonance Electronic spectroscopy: Energy levels, orbital and spin selection rules, vibronic transitions, polarizations. Vibrational progressions. Franck-Condon principle (quantum mechanical formulation), geometry of the excited states.

Polarisation of Raman lines, mutual exclusion principle and its application to molecular structure determination. Resonance Raman, Hyper-Raman, and stimulated Raman effect.

02 Resonance Spectroscopy (NMR and EPR) (15 – 20 lectures)

Nuclear energy levels in a magnetic field, nuclear magnetic resonance (NMR) and its instrumentation; Bloch equations and their solutions; chemical shift and nuclear shielding (diamagnetic and paramagnetic), fine structure and spin-spin interaction shape of spectral lines, spin-lattice relaxation time and line width. Echo experiments, NMR of solids, NMR imaging, Elementary idea of CIDNP.

Energy levels of a spinning electron in a magnetic field, principle of EPR spectroscopy and instrumentation. X-band and Q-band spectra, linewidth, hyperfine splitting, g-anisotropy and hyperfine splitting. EPR of triplet states, EPR spectra of paramagnetic salts and organic radicals (some typical examples), spin-orbit interaction and symmetry of crystal field, EPR and delocalization of spin. Elementary idea of CIDEP.

03 Electrical and Magnetic Properties (15 – 20 lectures)

Limitations of Debye equation. Curie-Weiss point and ferroelectricity; Onsager's theory of internal field, Kirkwood's equation and structure of water, dielectric dispersion and loss. Dielectric effect on emission and absorption spectra, Lippert-Mataga equation and structure of water, dielectric dispersion and loss. Dielectric effect on emission and absorption spectra, Lippert-Mataga equation, frequency dependent dielectric property. Debey semi-circle, relaxation time,deviations from Debye's theory, time resolved spectroscopic studies and dielectric relaxation effect. Quantum mechanical theories of dia-and para-magnetism, anisotropy, ferro-and antiferro-magnetism.

04 Photochemistry (15 – 20 lectures)

Sequence of processes in a photochemical reaction, deactivation of the excited state through different processes; fluorescence, phosphorescence, delayed fluorescence, resonance fluorescence, fluorescence quenching, determination of radiative lifetime of the excited state-principle and instrumentation, ground and excited state complexation. Franck-Condon principle and mirror symmetry.

Laser : principle, properties, and examples (solid state laser, dye laser, gas laser, excimer laser), application of laser radiation in supersonic jet spectroscopy, surface second harmonic generation (SSHG), salvation dynamics, excited state proton transfer and excited state acidity, and laser flash photolysis (with applications).

05 Principles of FT NMR Spectroscopy and Reaction Dynamics (15 – 20 lectures)

FT NMR Spectroscopy : Fourier transformations (general idea) time domain versus frequency domain, introduction to FT NMR spectroscopy, origin of chemical shift, factors which influence chemical shift, spin-spin splitting, 2D methods, application to structure analysis (simple cases).

Reaction Dynamics : General introduction, molecular dynamics intermolecular collision and its consequence: role of intermolecular potential, collision cross section, reaction cross section, energy threshold, reaction probability. Angular distribution in reactive collisions. Scattering in velocity space, electronic energy transfer. Experimental methods-crossed molecular beams. Photo-fragmentation spectroscopy, femtochemistry.

Paper VIII FM – 75
Physical Chemistry Special
Polymer Science

Unit

01 **High polymer system** **(15 – 20 lectures)**

Basic principles, definition, origin and classification of polymers, structure-property relationship. Rubbers, plastic and fibres. Polymer characterization : End groups, head to tail structure. Molecular weight and molecular weight distribution. Number average, weight average and viscosity average molecular weight fraction of polymers; polydispersity index.

02 **Step growth and Condensation polymerization** **(15 – 20 lectures)**

Functionality principles, kinetics and mechanism of step growth of polymerisation systems. Molecular weight control in linear stepwise polymerization. Molecular weight distribution in condensation polymers. Carothers equation and Flory equation, prediction of gel point.

03 **Chain Growth or Addition polymerisation** **(15 – 20 lectures)**

Free radical and ionic (cationic and anionic) polymerisation and their kinetics and mechanism; degree of polymerisation and its control, chain transfer, copolymerisation, steroregular polymerisation. Techniques of polymerisation. Mass, solution, suspension, and emulsion polymerisation.

04 **Plastics Technology** **(15 – 20 lectures)**

Materials: Synthesis, properties, uses and applications of-polyethylene, polypropylene, ethylene copolymers, polystyrene, polyvinyl chloride, acrylics, acetal resins, cellutosics, polycarbonates phenol-formaldehyde resins, alkyd resins, linear and fibre forming polyesters, nylon polyamides, epoxy resins.

Processing technology : polymer additives, mixing and compounding.

05 **Rubber Technology** **(15 – 20 lectures)**

Materials, Natural rubbers, styrene-butadiene rubber (SBR), polychloroprene, polybutadiene, nitrile rubber, ethylene-propylene rubber, EPDM rubber, chlorosulfonated polyethylene (Hypalon), polysulfide rubber, butyl rubber.

Silicone resins and rubbers: synthesis, properties, uses and applications.

Books Recommended :

(1) Physical Chemistry : Berry, Rice and Ross
(2) Physical Chemistry : Moore
(3) Physical Chemistry : Atkins
(4) Physical Chemistry : Levine
(5) Chemical Kinetics : Laidler
(6) Kinetics and Mechanism : Frost and Pearson
(7) Thermodynamics of Irreversible processes; Prigogine
(8) A Treatise on Heat : Saha and Srivastava
(9) Quantum Chemistry : Eyring, Walter and Kimbal
(10) Quantum chemistry : Pilar
(11) Quantum Chemistry : Levine
(12) Electrochemistry : Glasstone
(13) Electrochemistry : Bockris and Reddy
(14) Molecular Spectroscopy : Banwell
(15) Molecular Spectroscopy : Barrow
(16) Molecular Spectroscopy : Grabeal
(17) Molecullar Spectroscopy : Chang
(18) Group Theory : Bishop
(19) Group Theory : Cotton

(20) Group Theory : Hammermesh
(21) Molecular Spectroscopy : Levine
(22) Introduction to NMR Spectroscopy : Slichter
(23) Introduction to FT-NMR. Derome
(24) Electrol Spin Resonance in Chemistry : Aeyscoth
(25) Chemical Kinetics and Molecular Dynamics : Billing and Mikelson
(26) Introduction to Solid State Physics : Kittel
(27) Introduction to Statiscal Thermodynamics : Hill
(28) Introduction Statistical Mechanics : Hill
(29) Introduction to Statistical Mechanics : Pathria
(30) Biochemistry : Voet and Voet.

M.Sc. Part – II
(Physical Special) Practical

Unit

01 **List of Experiments :**

(1) Determine the order and rate constant of the reaction between $K_2S_20_8$ & kI and study the influence of ionic strength on the rate constant (two days).

(2) Conductometric determination of concentrations of KCI, HCI and NH_4Cl in a mixture (one day).

(3) Study of the Kinetics of alkaline hydrolysis of crystal violet. Determine the order with respect to alkali and salt effect on the system (two days).

(4) Determine the indicator constant of bromocresol green spectrophotometrically (one and half day).

(5) Determine the rate constant of alkaline hydrolysis of an ester (e.g., methy I acetate, etyl acetate, etc.) conductometrically (one day).

(6) Determine the dissociation constants (K_1, K_2, K_3) of H_3PO_4 by pH-meter (one day).

(7) Verify the Onsagar equation using KCI, K_2SO_4, $Bacl_2$ as electrolytes and determine their A values (one and half day)

(8) Determination of rate constant at different temperatures for the decomposition of H_2O_2 by acidified Kl solution and hence determine the activation energy of the reaction (two days).

(9) Potentiometric titration of halide mixture (chloride, bromide and iodide).

(10) Study the phase diagram of three component liquid system (benzene-acetic acid water/chloroform-acetic acid water) (one day).

(11) Determine the E value of Ag/Ag electrode and activity coefficients of different aqueous $AgNO_3$ solutions potentiometrically (one day).

(12) Determine the rate constant and order of the reaction of $KBrO_3$, & Kl in acid medium (one and half day).

(13) Determine the standard potential of $Fe(CN)_6^{3}/Fe(CN)_6^{4}$ electrode by potentiometer (one day).

(14) Determine the equilibrium constant of hydrolysis of an ester (e.g. methyl acetate, ethyl acetate, etc.) in acide medium (Two days).

(16) Determination of isoelectric point of a protein by viscosimetric method (one day).

(17) Determination of CMC of a surfactant in aqueous solution by conductometric method (one day).

(18) Study of the kinetics of iodination of acetone in presence of acid colorimetrically and hence find out the rate constant, order of reaction with respect to both the reactants and overall order and/or salt effect and effect of pH on kinetics (one and half day).

(19) Determination of dipole moments of solute and solvent by measuring the capacitance (one day).

(20) Determination of composition of complexes (ferricsalicylate complex/ ferrous-orthophenthroline complex) by Job's method (one day)

(21) Determination of partial molal volume.

(22) Determination of hydrolysis constant of a salt (e.g., aniline hydrochloride, NH_4cl. etc.) by conductometric/pH-metric/distribution method (one day).

At least eighteen (18) experiments are to be performed by a student of M.Sc. Part-II (Physical special)during the laboratory session.

Practical Examination of M.Sc.
Pat-II Physical Special :

Unit 01 :

Physical chemistry Experiments [Three days (Six hours each day) examination].

Total Marks : 105 (one hundred and five only).

A student has to perform (1) three experiments each of one day duration, or (2) two experiments each of one and half day duration, or (3) two experiments of which one is of one day duration and the other one is of two day duration.

Unit 02 : Internal Assessment

Total Marks : 30 (thirty only).

Unit 03 : Viva-voce and Laboratory Note Book (during examination)

Total Marks : 15 (fifteen only).

M.Sc. Part-II
PROJECT WORK/PROFESSIONAL SUBJECT PRACTICAL
(Physical Special)
Full Marks = 50, 30 – 40 days (3 hours per day).

Unit

01. Topics of investigation to be assigned by instructor/class teacher

Durating of work will 30 – 40 days (3 hours per day). Students have to submit the report of his/her work in the form of a Thesis (in duplicate). Thesis will be adjudicated jointly by a board of examiners consisting of the one internal and one external examiners . [30]

02. Viva-Voce

To be conducted jointly by the internal and external examiners on the thesis submitted under **01** [10]

03. Seminar

Every student has to deliver a seminar lecture (20 -30 mins duration) in the department on topics assigned by the class teacher or on any topics in chemistry of contemporary interest. Evaluation will be done by the class teacher based on individuals performance in the seminar.

M.Sc. Part- II

Organic Chemistry (Special)

Paper V

(Every unit consists of 15 lectures; Full Marks = 75)

Unit

01 Linear Free Energy Relationships :

Quantitative correlations of rate and equilibria. Linear free energy relationships with special reference to Hammett. Taft, Yukawa-Tauno and Grunwald-Winstem equations. Applications to aromatic, aliphatic polynuclear and hetero-atomic systems. Multiparameter correlation reactions (elementary ideas). Electrophilic substitutions in aliphatic systems (S_E1 and S_E2 reactions).

02 Pericyclic reactions and applications of MO theory to Organic Chemistry :

Electrocyclic reactions, Sigmatropic rearrangements, cycloaddition and cycloreversion reactions, cheletropic reactions, ene reaction, Frontier Molecular Orbital theory, concept of aromaticity of Transition States, orbital correlation diagrams, Huckel MO theory – MO's of chains and rings, alternants and nonalternants.

03 Stereochemistry – I: Conformational Aspects

Stereochemistry of rings :4-10 membered rings, fused ring systems, decalins, perhydroanthracenes and their conformations. β – strain, α - strain allylic 1,3-strain, stereochemistry of tricovalent carbon.

04 Stereochemistry – II : Other aspects :

Qualtitative treatment of mobile systems. Curtin Hammett principle. Asymmetric synthesis, stereoselectivity, O.R.D. and C.D. spectra, axial haloketone rule. Octant rule.

05 Organic Photochemistry :

Fundamental concepts, Jablonski diagram, Photochemistry of organic compounds : Norrish type – I and type – II processes, Patterno Buchi reaction, Barton reaction addition reaction, oxidation reaction, reduction reaction, substitution reaction, cis-trans isomerism, photochemistry of butadiene, Di-pi methane rearrangement and related processes.

M.Sc Part – II

Organic Chemistry (Special)

Paper – VI

(Every unit consists of 15 – 20 lectures; Full Marks = 75)

Unit

01 **Organic synathesis, Strategy and Organometallic Chemistry** :
Retrosynthetic analysis, the disconnection approach, use of transition metals: organometallics in organic synthesis. Preparation and reactions of pi-complexes, heptonumbers, rules for nucleophilic addition to pi-complexes, applications to typical synthesis.

02 **Heterocycles : Synthesis and Reactions :**
Generalized approach to the synthesis of hererocycles possessing 5-, 6- and 7- membered rings with one ro two heteroaatoms per ring. Reactions of heterocyles: oxidation and reduction reactions with electrophiles, nucleophiles and other reactive intermediates with typical monocyclic and fused ring systems as examples.

03 **Bioorganic Chemistry :**
Crown ethers, cryptands, molecular recognition. H-bonding in molecular organization, chiral recognition, Cyclodextrins. Introduction to molecular mechanics calculation and its use in the design of molecular receptors.
Enzymes : enzyme-kinetics and mechanism, application of enzymes in organic synthesis, enzyme model applications, enzyme models based on cyclodextrins, micelles, reverse micelles.
Chemistry of nucleosides, nucleotides and ATP, elementary structure and role of DNA and various types of RNA's in protein biosynthesis.

04 **Supramolecular Chemistry :**
Self-replication, Self-assembling systems. Gels, liquid crystals, molecular electronic devices, organic conductors, photoresponsive systems, chemical sensors.

Structure and conformation of protein and polysaccharides, biological roles of protein and polysaccharides in immunochemistry.

05 **Biologically Active Molecules :**
Antibiotic, vitamins and coenzymes : Synthesis and structure, biosynthesis, transformation reactions and biological activities of Antibiotics : penicillin, cephalosporin, streptomycin, chloramphenicol, Vitamins : A, B group, C and K, Coenzymes : NAD, FAD cocarboxylase, coenzyme A.

References :

(1) Bioorganic Chemistry, H.Dugas
(2) Bioorganic Chemistry, H. Dugas, .. Penny
(3) Bioorganic Chemistry Frontiers, Vol. 2
(4) Supramolecular Chemistry, J-M Lehn.
(5) Nobel Lecture, D.J.Cram.

M.Sc. Part-II

Organic Chemistry (Special)

PAPER – VII

(Every unit consists of 15 lectures; Full Marks = 75)

Unit

01 **NMR Spectroscopy :**

Principles, Relaxation phenomenon, factors influencing chemical shifts and coupling constants, simplification of complex spectrum, NOE, Rotating frame of reference. Detailed study of HNMR and preliminary aspects of CNMR, CW and FT techniques.

02 Mass-spectrometry combined applications of spectroscopical methods to organic molecules

Principles of Mass spectrometry. Different techniques, fragmentation modes. Combined application of spectroscopic techniques (UV, IR, NMR, MS) in elucidation of structure and study of reactions of organic compounds.

03 **Alkaloids**

Indole alkaloids – biogenesis and chemistry of representative members such as yohimbine, reserpine, strychnine, other alkaloids: quinine, morphine and its derivatives.

04 **Acetogenins, Prostaglandins and Porphyrins**

Structure, reactions, synthesis and biosynthesis of typical prostaglandins. Biogenesis and chemistry of acetogenins – Coumarins, flavanoids, lignan and porphyrin, some typical examples.

05 **Terpenes and Steroids**

Biogenesis of terpenoids and steroids. Structure elucidation and synthesis of some representative members of monosesqui, di-and tri-terpenoids from the following : Logamin, Santonin, Germacrane, Zerumbone, farnesol, gibberalline, caryophyllene, abietic acid, squalene, presqualene, amyrins and lypeols.

Steroids nomenclature, representative members such as cholesterol, sex hormones and artificial hormones.

M.Sc. Part – II

Physical Chemistry / Organic Chemistry Special

Paper – VIII, Polymer Science

(Every unit consists of 15 lectures : Full Marks = 75)

Unit

01 **High Polymer System**

Basic principles, definition, origin and classification of polymers, structure-property relationship. Rubbers, plastic and fibres. Polymer characterisation : End groups, head to tail structure. Molecular weight and molecular weight distribution. Number average, weight average and viscosity average molecular weight fraction of polymers : polydispersity index.

02 **Step growth and Condensation polymerisation**

Functionality principles, kinetics and mechanism of step growth of polymerisation systems. Molecular weight control in linear stepwise polymerisation. Molecular weight distribution in condensation polymers. Carothers equation and Flory equation, prediction of gel point.

03 **Chain Growth or Addition polymerisation**

Free radical and ionic (cationic and anionic) polymerisation and their kinetics and mechanism, degree of polymerization and its control, chain transfer, copolymerisation, stereoregular polymerisation. Techniques of polymerisation. Mass, solution, suspension and emulsion polymerisation.

04 **Plastics Technology**

Materials Synthesis, properties, uses and applications of – polyethylene, polypropylene, ethylene copolymers, polystyrene, polyvinyl chloride , acrylics, acetal resins, cellutosies, polycarbonates, phenol-formaldehyde resins, alky resins, linear and fibre forming polyesters, nylon polyamides, epoxy resins.

Processing technology : polymer additives, mixing and compounding.

05 **Rubber Technology :**

Materials, Natural rubbers, styrene-butadiene rubber (SBR), polychloroprene, polybutadiene, nitrile rubber, ethylene-propylene rubber, EPDM rubber, chlorosulfonated polyethylene (Hypalon), polysulfide rubber, butyl rubber .

Silicon resins and rubbers : synthesis properties uses and applictions.

PRACTICAL

(Organic Special)

Full Marks : 150, three days (6 hours per day)

Unit

01 Separation followed by systematic qualitative analysis of two component mixture or two solids. Pure samples of the compounds and their suitable crystalline derivatives are to be submitted along with proof of their purity (by TLC or paper chromatographic analysis). At least 5 mixtures to be analysed. [30]

02 Qualitative Analysis of an organic liquid substance leading to its identification [20]

03 Preparation of organic compounds by typical multistep procedure (a least four synthetic sequences to be performed). Samples of final product and intermediates to be submitted. UV, and IR spectra of products to b recorded and interpreted. [30]

04 Quantitative Analysis by Chemical and UV-Vis spectrophotometry. Estimation of functional groups, nitrogen (semi-micro/microkjeldah method). Drug analysis (At least four analysis to performed).

05 Chromatographic separation techniques (paper, thin layer, column) qualitative and/or quantitative.

06 **Sessional**

To be awarded by the class teacher on the basis of performance durin course work.

07 **Viva-Voce** (during examination)

To be conducted jointly by the internal and external examiners.

M.Sc. Part – II

PROJECT WORK/PROFESSIONAL SUBJECT

PRACTICAL

(Organic Special)

Full Marks = 50, 30-40 days (3 hours per day).

Unit

01 **Topics of investigation to be assigned by instructor/class teacher**

Duration of work will 30-40 day (3 hours per day). Students have to submit the report of his/her work in the form of a Thesis (in duplicate). Thesis will be adjudicated jointly by a board of examiners consisting of the one internal and one external examiners. [30]

02 **Vica-Voce**

To be conducted jointly by the internal and external examiners on the thesis submitted under **01** [10]

03 **Seminar**

Every student has to deliver a seminar lecture (20-30 mins duration) in the department on topics assigned by the class teacher or on any topics in chemistry of contemporary interest. Evaluation will be done by the class teacher based on individuals performance in the seminar. [10]

M.Sc. Part – II

PAPER – V

INORGANIC CHEMISTRY

(Every unit consists of 15 – 20 lectures, Full Marks = 75)

Unit

01 Application of Group Theory

Symmetry of orbitals. Symmetry Adapted Linear Combinations— LCAO-MO. Hybrid orbitals (O_h T_d). Molecular Orbitals (O_h T_d) Correlation diagram and interpretation of Tanabe Sugano diagram, Molecular vibration and vibrational transitions.

The general variational procedure, ab-initio calculation of M.O. and energy levels of H_2 ion. Born-Op[enheimer approximation and molecular hamiltonian. Concept of charge density/bond order. Preliminary discussions on semiempirical MO Mulliken – Wolfsberg – Helmoltz method (examples of H and/or MnO_4).

02 Coordination Chemistry : Structure and Bonding

Valency bond VSEPR model. Calculation of ideal (theoretical) interbond angles. Qualitative assessment of repulsion of bond pair and nonbond pair of electrons on the angular distortion. Examples.

Isomerism in coordination compounds. Optical activity, absolute configuration and enantionmers. CD, ORD & MCD Cotton and Faraday effects. Racemisation. Ray-Dutt and Bailar mechanisms.

03. Inorganic reaction mechanism

Substitution reactions : Thermodynamic and kinetic consideration of steady state and equilibrium, stoichiometry and rate law, activation parameters (H S, V) thermodynamic and kinetic stability.

Experimental methods : Slow and Fast reactions. Spectrophotometry, stopped flow, T-jump.

Classification of mechanisms: A,D,I,I_a I_d .

Factors determining the mechanism: electronic structure of metal ions, crystal field effect, nature of entering species. Examples of Co(III), Cr(III) and Ru(III) octahedral complexes. Twist mechanisms Pt(II) square planar complexes, trans effect.

Electron transfer reactions: Atom transfer and electron transfer processes. Mechanism of electron transfer reactions — Outer sphere (mechanism, cross section and thermodynamics); Mercus theory; Inner sphere I conditions, formation of precursor complexes, fission of successor complexes) Induced electron transfer processes, two electron transfer.

04. Magnetochemistry and EPR spectroscopy.

Magnetic properties of substances, orbital and spin moments (electrons), paramagnetism and magnetic susceptibility. Curie and Curie – Weis law with derivation. Van Vleck theory – derivation of Van Vleck equation and its application (energy difference between energy levels – smaller, comparable and larger than k T). Temperature Independent Paramagnetism(TIP).

Magnetic properties of free ions ——First order and second order Zeeman effect. Effect of spin orbit coupling. Examples (Sm_{3+}, Eu_{3+}).

Magnetic properties of metal complexes —— Quenching of orbital angular momentum for A.E.T terms and magnetic properties under Oh and Td field. Examples and calculation of in selected cases. Antiferromagnetic interaction in Inorganic compounds. Mechanisms — direct interactions, super exchange interactions. Antiferromagnetic Interactions in polynuclear complexes.

Electron Paramagnetic Resonance Spectroscopy – Application in coordination chemistry with special to the determination of oxidation state of metal ion in complexes. Magnetic exchange in polynuclear complexes etc.

05. Application of spectroscopic techniques in inorganic chemistry.

NMR/FT-NMR : $^{11}B^{19}$. $F.^{15}$ V^{1} and ^{31}P NMR spectra in detection and structural studies of Inorganic compounds — Phosphorous acids, phosphates (including ply phosphates) P.S. ring compounds. Boron polyhedral compounds. B-N compounds. Fluorides and Fluoro complexes. NMR of paramagnetic species.

Application of IR/FT-IR in Coordination Chemistry (H_2O,NH_3 CO, CN, ClO_4, SCN)

Principle and application of Mossabaur spectroscopy in Inorganic Chemistry.

Photoelectronspectroscopy. NQR spectroscopy.

Structure elucidation of simple inorganic molecules.

M.Sc. Part-II, PAPER – VI

INORGANIC CHEMISTRY

(Every unit consists of 15 – 20 lectures, Full Marks = 75)

Unit

01 Organometallic Chemistry.

Stability of Organometallic compounds – Main group and Transition metal. Chemistry of M-C σ bonded compounds N-C double bonded compounds (carbenes and alkylidines), M-C triple bonded compounds (alkylidenes) synthesis, structures, bonding and reactivity.

Chemistry of transition metal complexes incorporating olefinic and acetylenic ligands. Open chain conjugated ligands up to 5 carbon atoms containing chains.

Chemistry of transition metal complexes with cyclic polyenes 3-6 membered ring system. Sandwich and non sandwich complexes (bent Cp-rings).

Organometallic Chemistry of hetero cyclic ligands (N.B.O) Multidecker sandwich complexes.

02 Catalysis

Reactions in organometallic chemistry and catalysis – cooddanitev unsaturation, ligand dissociation and substitution. Oxidative addition, insertion (migration) and reductive elimination reactions.

Alkene insertion and isomerisation.

Homogeneous catalytic processes – catalytic efficiency and energetics. Alkene hydrogenation, water gas shift reactions. Fischer-Tropsch process. Hydro formylation (Oxo process), caboxylation of olefins. Monsanto's acetic acid synthesis, Wacker oxidation (palladium catalysed).

Polymerization of olefins – Ziegler Netta catalyst.

03 Metal carbonyls, Metal Clusters and M-M multiple bonds

Metal carbonyls – synthesis, structure and reactivity. Low nuclearity (M_3 M_4) and high nuclearity (M_5 M_{10}) carbonyl clusteres.

Metal-metal bonding (MO), skeletal electron counting. Wade-Mingos-Lauher rule, isolobal analogy.

Halides clusters of Nb, Ta, Mo, W, Re. Synthesis structures and bonding.

Interstitial Clustures – hydrides, carbides and nitrides.

Metal – Metal multiple bond. Examples, synthesis, structures and bonding (MO). Electronic transition.

04 Bioinorganic Chemistry

Ion transport across membrane – Na -K pump. ATPase. Nonhernme O_2 carrier – Hemerythrine and hemocyanine. Copper transport protein – Ceruloplasmin, Wilson's disease. Electron transfer (redox) enzymes – Cytochrome c oxidase, Cytochromr P^{45} Catalase peroxidase. Ascorbate oxidase and Superoxide dismutase. Respiratory electron transport chain. Hydrolytic enzymes – Carbonic Anhydrase, Carboxy peptidase, Hydrogenase, Urease.

Vanadium containing proteins – Amavadin, Vanadium bromoperoxidase. Vitamin B_{12} Chlorophyl (Photosystem).

05 Chemistry of f-block elements

Lanthanides. Actinides and Super heavy elements. Electronic structure, difference between 4f and 5f orbitals. Stable oxidation states. Lanthanide and Actinide construction, separation and isolation. Absorption spectra and magnetic properties.

Comparative chemistry of d and f block elements. Comperative chemistry of Lanthanides and Actinides. Aqueous chemistry, coordination chemistry. Organometallic compounds, trans actinide elements, nuclear instability and Synthesis chemistry of U and Pu. Periodicaity of trans L awrencium elements superactinides.

M.Sc. Part-II

PAPER – VII

INORGANIC CHEMISTRY

(Every unit consists of 15-20 lectures, Full Marks = 75)

Unit

01 Solid state

Theories of bonding in solids ——— Free electron theory of metals. Fermi surface. Brillouin zone and density states. Hall effect, electrical and thermal properties of metals. X-ray crystallography —— Crystalline solids: single and polycrystals. Crystal lattice and lattice structures (primitive and monprimitive unit cells).

Crystal symmetry : Point group elements and space group elements. 32 crystal classes. HM notations, stereographic projections.

Space lattice : Different plane lattices, additional symmetry elements and possible stacking to generate space lattices, 14 Bravais lattices and their distribution.

Space group : HM notation, different space groups in triclinic and monoclinic systems.

X-ray diffraction: necessary condition, L au equation, equivalent reflections. Reciprocal lattices, sphere of reflection and lattice parameters.

Structure solutions : Introduction to direct and heavy atom (Patterson) method for structure solution from x-ray data obtained from single crystal x-ray diffractometer.

02. Inorganic photochemistry

Excited states: Ligand field, charge transfer, Frank-Condon. THI:XI and DOSENCO states. Relaxation processes. Photophysical and photochemical processes. Kinetics of photochemical processes. Reactivities of transition metal complexes in ligand field excited states (d3 and d6 systems) and charge transfer excited states with reference to substitution and electron transfer reactions. Photosensitisers. Application of inorganic photochemical processes. Photochemical splitting of water.

Photochemistry of Organometallic and metal-metal multiple bonded species. Bonding in metal-metal multiple bonded species and charge transfer process.

03. Analytical methods

Solvent extraction separation methods. Chromatographic and ion-exchange separation techniques. Examples.

Electroanalytical methods : Polarography — polarised and depolarised electrodes, diffusion currents, Ilkovic equation (simplified derivation) and its significance. Current—— potential curve and its application.

Cyclic voltametry and Coulometry — Basic principle, three electrode configuration, solvents and supporting electrolytes, Representation of cyclic voltammogram, half wave potential, irreversible, reversible and quasireversible redox processes. Electron transfer at a constant potential, no. of electron transfer. Applifation in coordination chemistry (characterisation, determination of redox potential). Examples (ferrocene, Co(II)/Co(III); Ni(II)/Ni(III), Cu(I)/CU(II);Ru(II)(bpy).

Thermal methods of analysis : Basic principles of Differential Thermal Analysis, Thermo Gravimetric Analysis. Applications in coordination chemistry.

04. Geochemistry, Marine Chemistry and Corrosion Chemistry

Geochemistry : Geochemical structure and composition of the earth; distribution of elements; mineral formation and deposits; origin of coal and petroleum.

Marine Chemistry : The sea – water equilibria; pressure and temperature gradient: pH and pE of sea water; salinity and chlorinity, methods of salinity and chlorinity measurements; Major and minor elements in sea water; phosphorus and nitrogen cycles.

Corrosion: Corrosion is an electrochemical phenomenon (experiments): Examples of corrosion in atmospheric, marine and underground environment. Pourbaix potential. Pl I diagram for understanding corrosion.

05. Some aspects of advanced inorganic Chemistry

Syntheses and structure of polynuclear transition metal complexes — formation of dendrimners.

Ligand based redox systems — dioxolene, ditiolene, diimine and iminophenolate complexes. Characterisation and structural features.

Stabilisation of uncommon oxidation states of transition metals by complex formation -=— Fe(IV), Co(IV), Ni(III), Ru(IV), Os(IV), Pd(III), Pd(IV), Pt(III), Syntheses and structures.

Interaction of metal ions with nuceic acids. Replication, transcription. Antitumor drug.

M.Sc. Part-II,

PAPER – VIII

INORGANIC CHEMISTRY

Professional Course (Environmental Chemistry)

(Every unit cosists of 15-20 lectures, Full marks = 75)

Unit

01 Environmental Segments

Chemistry of Atmosphere : Structure, Composition evolution, earth's radiation balance. Particles, gasesions and radicals in the atmosphere. Chemical and photochemical reaction, green house effect.

Chemistry of Lithosphere : Composition, inorganic and organic components, macro and micro nutrients, C, N, O, P and S cycles.

Chemistry of the Hydrosphere : Hydrologic cycle, Physical C hemistry of sea water, carbonate – bicarbonate buffer system, complexation and microbial reactions in waster water, Eutrophication.

02 Environmental Pollution

Air Pollution : Primary pollutants and their origins, harmful effects of Co, NO_8, SO_8, hydrocarbons and other organic, photochemical smog, CFC's, ozone whole, particulate matters, acid rain, radioactive pollutants and their effects.

Water Pollution : Aquatic pollutants, chemical, radioactive and thermal pollution, basic gaseous and coloured inorganic and organic pollutants, Pollutants in industrial effluents and sweage, Fertilizer waster, agricultural run off, pesticides and other pollutants in the soil.

Solid waste : Treatment and disposal of solid waster, Municipal garbage waste, waste from power plants etc.

03. Chemical Toxicology

Trace elements and their chemical speciation with special reference to Cu, Zn, Cd, Hg, P, Ag, Sb, Se, Tl, Si, Be etc. Toxic chemical in air, water, soil, diet, fertilizer, their effects and remedial measures.

Metal ion toxicity, metal dependent diseases, remedial measures, Biomineralogy.

04. Environmental Analysis

Air quality standard, sampling and monitoring, detection and determination of CO, SO_2, NO_3, H_2S Hydrocarbon and particulate metters.

Water quality standard, sampling and monitoring, determination of pH. Conductance, hardness, total dissolved solid, dissolved oxygen, COD, BOD, metallic ions and anions and organic particulate matters.

Applications of Chromatographic techniques, gas chromatography, gas – liquid chromatography, spectrophotometry, IR and NMR spectrometry., polarographic and voltametric methods, atomic absorption spectrometry in environmental analysis.

05 Pollution control measures :

Removal of particulate matter, CO, SO_2, NO_3, H_2S and organics from air, treatment of auto exhaust and few gases, cyclone separators, electrostatic precipitators, absorption and absorption and combustion techniques.

Removal acidic, basic, inorganic and organic, audorons and coloured pollutants from water, chemical and microbial method. Treatiment of Industrail efluents from alkali, chlorine, paper, jute, textile, leather, cement, rubber plastic, fertilizer electroplating industry, steel plant, thermal poser plant, radioactive waster dispotal, domestic sewage and agricultural run off. Water treatment, municipal and industrial water. Drinking water from sea. Removal of hardness, Chemical and electrochemical methods, coagulation, electro coagulation, ion exchange, reverse osmosis, electro dialysis methods.

M.Sc. Part – II
(PRACTICAL)
(Inorganic Special)
Full Marks 150, three days (6 hours per day)

i. Preparation of typical Inorganic Compounds (simple and complex) and their characterisation by analysis, spectra, magnetic and conductance data. [20]

ii. Quantitative anlysis of complex materials. Ores and minerals (dolomite, bauxite, chromite, pyrolusite etc.), alloys (ferrous and nonferrous) by volumetric/gravimetric/colorimetric methods [40]

iii. **Physicochemical experiments** (any five experiments) [40]

a. Colorimetric determination of composition of metalligand complexes (slope ratio/moleratio/Job's method)

b. Determination of protion-ligand and metal-ligand stability constants by pH metric method.

c. Determination of molar conductance values of simple and complex inorganic compounds and characterisation of electrolyte type.

d. Conductometric study of the reaction of inorganic compounds and determination of rate constants.

e. Study of electronic spectra of transition metal complex, verification of spectrochemical and nephelauxetic series.

f. Kinetic study of ligand displacement reactions.

iv. **Sessional** [30]

To be awarded by the internal teacher on the basis of preformance during course work.

v. **Viva-voce** [20]

To be conducted by the internal and external examiners jointly.

M.Sc. Part-II
PROJECT WORK/PROFESSIONAL SUBJECT PRACTICAL
(Inorganic Special) (Full Marks=50, 30-40 days (3 hours per day)

Unit

01 **Topics of investigation to be assigned by instructor/class teacher.**
Duration of work will 30-40 day (3 hours per day), Students have to submit the report of his/her work in the form of a Thesis (in duplicate). Thesis will be adjudicated a jointly by a board of examiners consisting of the one internal and one external examiners [30]

02 **Via-Voce**
To be conducted jointly by the internal and external examiners on the thesis submitted under 01. [10]

03 **Seminar**
Every student has to deliver a seminar lecture (20-30 mins duration) in the department on topics assigned by the class teacher or on any topics in chemistry of contemporary interest. Evaluation will be done by the class teacher based on individuals performance in the seminar [10]

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