JAMSHEDPUR WOMEN'S COLLEGE

(A CONSTITUENT AUTONOMOUS COLLEGE OF KOLHAN UNIVERSITY, CHAIBASA)

COLLEGE WITH POTENTIAL FOR EXCELLENCE BY UGC, NEW DELHI, JAMSHEDPUR-831001

"A GRADE COLLEGE BY NAAC

DEPARTMENT OF CHEMISTRY

SYLLABUS

FOR

FACULTY OF SCIENCE

M.SC.(CHEMISTRY) PART-1 & PART-11

(2010 ONWARDS)

Proposed course of study for M.Sc. (Part I & II)

Outline of curricula M.Sc. (Chemistry)

There will be 600 marks in each semester I, II, III and IV. In I, II and III semester there will be four theoretical papers in each semester of 80 marks+internal assessment 15 marks + assignment 5 marks for each paper (total 100 marks for each theory paper).

Semester I and II in M.Sc. (Part I); Semester III and IV in M.Sc. (Part II) Semester I Practicai : Computer (100 marks)

Physical Chemistry (100 marks) Semester II Practical : Inorganic Chemistry (100 marks)

Environmental & Biochemistry (100 marks) Semester III Practical : Organic Chemistry (100 marks)

Analytical Chemistry (100 marks) Semester IV Practical : Special paper (100 marks)

(Organic, Inorganic and Physical) Semester IV Project work (100 marks) (Project-75 & Presentation-25) (Marks distribution In each practical paper-Experiment 70+NB10+W 20)

(Semester I), Paper 1

Inorganic Chemistry (80 marks)

Stereochemistry and Bonding in Main Group Compounds -

(30marks) 12Hrs.

VSEPR, Walsh diagrams (trl atomic molecules of type AH2) dn-pn bonds Bent rule and energetics of hybridization, some simple reaction of covalently bonded molecules .

Reaction Mechanism of Transition Metal Complexes

(30marks) 24Hrs.

Energy profile of a reaction, Reactivity of metal complexes, Inert and labile complexes, kinetic application of valence bond and crystal field theories, kinetics of octa hedral substation, acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, direct and Indirect evidences In favour of conjugate mechanism, anation reaction, reactions without metal ligand bond cleavage, Substitution reactions in square planar complexes, the trans

effect, mechanism of the substitution reaction, Redox recttons, electron transfer reactions, mechanism of one electron transfer reactions, outer sphere type reaction cross reaction and Marcus-Hush theory, Inner sphere type reactions.

Metal-Uoand Bonding : **(20marks) I5Hrs.**

Limitation of crystal field theory, molecular orbital theory, octa hedral, tetrahedral and square planar complexes, Tt-bonding and molecular theory.

Part-II (M. Sc.)
(Semester-I) Paper-2
Organic Chemistry (80 marks)

Unit : 1

Nature of bonding in Organic Molecules & Reaction Mechanism (15 Marks) 12 hrs.

Aromaticity In benzenoid and non benzenoid compounds. Alternate and non Alternate hydrocarbons, Huckel's rule. Energy level of pi Molecular Orbttals, annulenes, aiiti aromaticity, aromaticity, homo-aromaticity, PMO approach. Bonds weaker than covalent—addition compounds, crown ether complexes and cryptands, inclusion compounds, cyclodextrins, catenanes and rotaxanes.

Stereo Chemistry **(20 marks) 15 hrs**

Conformational analysis of cycloalkanes, decalins, steric strain due to unavoidable crowding. Elements of symmetry, chirality, molecules with one than one chiral center, threo and erythro isomers, methods of resolution, optical purity, enantiotopic and diastereotopic atoms, groups and faces, stereospecific and stereoselective synthesis. Asymmetric synthesis. Optical activity in the absence of chiral carbon (biphenyls, allenes and spiranes), chirality due to helical shape. Stereochemistry of the compounds containing nitrogen, sulphur and phosphorus.

Aliphatic and Aromatic Nucleophilic Substitution
(20 marks) 15 hrs.

The S_N1, S_N2, mixed S_Ni and S_N2 and SET mechanisms.

The neighbouring group mechanism, neighbouring group participation by π and σ bonds, anchimeric assistance.

Classical and non-classical carbocations, phenonium ions, norbornyl system, common carbocation rearrangements. Application of NMR spectroscopy in the detection of carbocations. The S_Ni mechanism.

Nucleophilic substitution at an allylic, allphatic trigonal and a vinylic carbon.

Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium, phase transfer catalysis and ultrasound, ambident nucleophile, regioselectivity.

Aliphatic and Aromatic Electrophilic Substitution :
(15 marks) 11 hrs.

Bimolecular mechanisms - S_E1 and S_E2. The S_Ei mechanism, electrophilic substitution accompanied by double bond shifts. Effect of substrates, leaving group and the solvent polarity on the reactivity. The arenium ion mechanism, orientation and reactivity, energy profile diagrams. The ortho\para ratio ipso attack, orientation in other ring systems. Quantitative treatment of reactivity in substrate electrophiles. Diazonium coupling, Vilsmeir reaction, Gattermann-Koch reaction.

Aromatic Nucleophilic Substitution **(10 marks)**

The S_NAr, S_N1, benzyne ans $S_{RN}1$ mechanisms. Reactivity - effect of substrste structure, leaving group and attacking nucleophile. The von Richter, Sommelet-Hauser and Smiles rearrangement.

M.Sc (Part 1
(Semester 1) Paper — 3
Physical Chemistry (80 marks)

Quantum Chemistry **(40 marks) 30hrs.**

A) Introduction to exact quantum mechanical results

The Schrodinger equation and the postulates of quantum mechanics. Discussion of solutions of the Schrodinger equation to some model systems viz. particle in a box, the harmonic oscillator, the rigid rotor, the hydrogen atom.

B) Approximate Methods

The variation theorem, linear variation principle. Perturbation theory (first order and non-degenerate). Applications of variation method and perturbation theory to the Hellum atom.

C) Angular Momentum

Ordinary angular momentum, generalized angular momentum, eigen functions for angular momentum, eigenvalues of angular momentum, operator using ladder operators, addition of angular momenta, spin, antisymmetry and Paul! exclusion principle.

D) Electronic Structure of Atoms

Electronic configuration, Russell-Saunders terms and coupling schames, Slater-Condon parameters, term separation energies of the pn configuration, term separation energies for the d" configurations, magnetic effects : spin-orbit coupling and Zeeman splitting, introduction to the methods of self-consistent field, the virial theorem.

E) Molecular Orbital Theory

Huckel theory of conjugated systems, bond order and charge density calculations. Applications of ethylene

butadiene, cyclopropenyl radical, cyclobutadiene. Introduction to extended Huckel theory.

Thermodynamics **(40 marks) 30 hrs.**

A) Classical Thermodynamics

Brief resume of concepts of laws of thermodynamics, free energy, chemical potential and entropies. Partial molar properties; partial molar free energy, partial molar volume and partial molar heat content and their significances. Determination of these quantities. Concept of fugacity and determination of fugadty. Non-Ideal systems : Excess functions for non-ideal solutions. Activity, activity co-efficient. Application of phase rule to three component systems; second order phase transitions.

B) Statistical Thermodynamics

Concept of distribution, thermodynamic probability and most probable distribution. Ensemble averaging, postulates of ensemble averaging. Canonical, grand canonical and microcanonical ensembles, corresponding distribution laws (using Langrange's method of undetermined multipliers).

Partition functions - translational, rotational, vibrational, electronic partition functions/calculation of thermo-dynamic properties in terms of partition functions. Applications partition functions.

Heat capacity behaviour of solids - chemical equilibria and equilibrium constant in terms of partition functions, Fermi-Dirac statistics, distribution law and applications to metal.

Bose-Einstein statistics-distribution law and application helium.

M.Sc (Part 1)
(Semester 1) Paper 4
Computer For Chemists (80 Marks)

Introduction to Computers and computing
(10 marks) 3 hr

Basic structure and functioning of computers with a PC as an illustrative example. Memory, I/O devices. Secondary storage Computer languages. Operating systems with DOS as an example Introduction to UNIX and WINDOWS. Data processing, principles programming. Algorithms and flow-charts.

Computer programming in C language
(30 marks) 20 hrs.

Elements of the computer language constants and variables ar data types. Operators and Expressions, Arithmetical, Relations Logical, Assignment, Increement and Decreement operators. Input and Output statements. Branching statements such as (if-else, got(switch) statements. Decision making and looping (while, for, do Arrays (one dimensional and two dimensional arrays). Sorting (data in an array. Function (user defined functions).

Programming in chemistry **(20 marks) 15 hrs.**

Development of small computer codes involving simple formulae in chemistry, such as Van der Waals equation. pH titration, kinetics, radioactive decay. Evaluation of lattice energy and lonic radii from experimental data. Linear simultaneous equations to solve secular equations within the Huckel theory. Elementary structural features such as bond lengths, bond angles, dihedral angles of molecules extracted from a database such as Cambridge database.

Use of computer programmes **(20 marks) 15hrs.**

The students will learn how to operate a PC and how to run standard programmes and packages. Execution of linear

regression, X-Y plot, numerical integration and differentiation as well as differential equation solution programmes. Monte Carlo and Molecular dynamics. Programmes with data preferably from physical chemistry laboratory. Packages-MS-Word, MS-Excel, FOXPRO, MATLAB.

M.Sc (Part 1)
(Semester 1) (Paper 5)
Practical - Computer

Time - 6 hrs. **Full marks: 100**

A) Familiarity and use of scientific packages such as Scientific Work Place (Scientific Word Processor), Spreadsheets, Database and Chem-X to solve problems in chemistry.

B) Modelling of typical case and its stimulation using Chem-X package.

C) Programming examples in C to handle the following problems in chemistry :

a) Least square fit

b) Solution of simultaneous equation

c) Polynomial equation and polynomial equation fitting

d) Matrix inversion and diagonalization

e) Empirical/molecular formula from elemental analysis

f) Molecular formula from mass spectroscopy

g) pH of a weak acid-base titration h) Potentiometric end point-titration

i) Monte Carlo stimulation of kinetics of a reaction and its energetics

j) Stimulation of Maxwell-Boltzmann distribution

k) R.M.S. Velocity and kinetic energy of a gaseous particle in 3-degree of freedom

I) Half-life period of nuclear decay

M.Sc (Part 1)
(Semester 1) (Paper 6)
Practical Physical

Time - 6 hrs. Full marks : 100 (40+40+NB10+W10)

A) Measurement of density of gases and vapours

a) Victor Meyer's Method

Determination of molecular weight of acetone, chloroform, benzene, (mixture).

B) Determination of Molecular weight of substances

a) Beckmann's freezing point method

C) Viscosity of liquids and solution by Ostwald tube

Determination of percentage composition of a mixture of two liquids

D) Surface tension of liquids and solutions

a) Determination of parachor

E) Thermochemistry

a) Determination of water equivalent of a calorimeter

b) Determination of the Heat of Neutralization of:

i) Weak acid and strong base (NaOH and CH_3COOH)

c) Determination of basicity of succinic acid by Thermochemical method

F) Order of reaction

a) Determination of the rate constant of hydrolysis of an ester with an acid (methyl acetate and HCL)

G) Partition Co-efficient

a) Determination of partition co-efficient of:

(i) Benzoic acid between water and benzene

H) Polarimetry

a) Study of inversion of cane sugar in acid medium

I) Conductivity

a) Determination of cell constant

b) Titration of:

(i) Strong acid and strong base (HCL and NaOH)

D) E.M.F.

a) Preparation of calomel electrode

b) Potiometric Titration of acid base

(M.Sc Part 1)
(Semester 2) (Paper 7)
(Inorganic Chemistry) (80 marks)

Metal ligand Equilibria in solution (10 marks) 8 hrs

Stepwise and overall formation constants and their interaction, trend;In stepwise constants, factors affecting the stability of metal complexes with reference to the nature of metal ion and ligand, chelate effect and its thermodynamic origin, determination of binary formatior constants by pH-metry and spectrophotometry.

Electronic Spectra and magnetic properties and transition metal complexes (30 marks) 24hrs.

Spectroscopic ground states, correlation, Orgel and Tanabe-Sugano diagrams for transition metal complexes (d^2-d^9 states), calculations of Dq, B and (B parameters, charge transfer spectra, Spectroscopic method of assignment configuration in optically active metal chelates and their stereochemical information, anomalous magnetic moments, magnetic exchange coupling and spin crossover.

Metal re-Complexes (20 marksT 18 hrs.

Metal carbonyls, structure and bonding, vibrational spectra of metal carbonyls for bonding and structural elucidation, important reaction of metal carbonyls; preparation, bonding, structure and important reactions of transition metal nitrosyl, dinitrogen and dioxygen complexes; tertiary phosphine as ligand.

Group Theory

A) Symmetry and group theory in chemistry **(10 marks) 12 hrs.**

Symmetry elements and symmetry operation, definitions of group, subgroup, relation between orders of a finite group and its subgroup. Conjugacy relation and classes. Point symmetry group. Schonflies symbols, representation of groups by matrices (representation for the Cn, Cnv, Cnh, Dnh groups to be worked out explicitly). Character of a representation. The great orthogonality theorem (without proof) and its importance. Character table and their use; spectroscopy.

B) Unifying principles **(10 marks) 10 hrs.**

Electromagnetic radiation, interaction of electromagnetic radiation with matter-absorption, emission, transmission, reflection, refraction, dispersion, polarization and scattering. Uncertainity relation and natural line width and natural line broadening, transition probability, results of the time dependent perturbation theory, transition moment, selection rules, intensity of spectral lines, Born-Oppenheimer approximation, rotational, vibrational and electronic energy levels.

M.Sc (Part 1)
(Semester 2) (Paper 8)
Organic Chemistry (80 marks)

Addition to carbon-carbon multiple bonds and carbon-hetero multiple bonds **(30 marks) 19 hrs.**

Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, region-and chemo-selectivity, orientation and reactivity. Addition to cyclopropane ring.

Hydrogenation of double and triple bonds, hydrogenation of aromatic rings. Hydroboration. Michael reaction. Sharpness asymmetric epoxidation.

Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters and nitrides. Addition of Grignard reagents, organozinc and organolithium reagents to carbonyl and unsaturated carbonyl compounds. Wittig reaction.

Mechanism of condensation reactions involving enolates-Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin and Stobbe reactions. Hydrolysis of esters and amides, ammonolysis of esters.

Elimination reactions **(20 marks) 15 hrs.**

The E2, El and EIcB mechanisms and their spectrum. Orientation i the double bond. Reactivity-effects of substrate structures, attackir base, the leaving group and the medium. Mechanism and orientatio in pyrolytic elimination.

Pericyclic reactions **(30 marks) 20 hrs.**

Molecular orbital symmetry, frontier orbitals of ethylene, 1,3 butadiene, 1/3,5-hexatriene and allyl system. Classification ofpericycli reactions. Woodward-Hoffmann correlation diagrams. FMO and PMO approach. Electrocyclic reactions-conrotatory and disrotator motions, 4n, 4n+2 and allyl systems. Cycloadditions-antrafacial and suprafacial additions, 4n and 4n+2 systems, 2+2 addition of ketenes 1,3-dipolar cycloadditions and chelotropic reactions.

Sigmatropic rearrangements - suprafacial and antrafacial of H sigmatropic shifts involving carbon moieties, 3,3- and 5, 5- sigmatropic rearrangements. Claisen, Cope and aza-Cope rearrangements Fluxional tautomerism. Ene reaction.

M.Sc (Part I)
(Semester II) (Paper 9)
Physical Chemistry (80 marks)

Chemical Dynamics **(30 marks) 20 hrs.**

Methods of determining rate laws, collision theory of reaction rates, steric factor, activated complex theory, Arrhenius equation and the activated complex theory; ionic reactions, kinetic salt effects, steady state kinetics, kinetic and thermodynamic control of reactions, treatment of unimolecular reactions.

Dynamic chain (hydrogen-bromine reaction, pyrolysis of acetaldehyde, decomposition of ethane). Photochemical (hydrogen-bromine and hydrogen-chlorine reactions) and oscillatory reactions (Belousov-Zhabotinsky reaction), homogeneous catalysis, kinetics of enzyme reactions, general features of fast reactions, study of fast reactions by flow method, relaxation method, flash photolysis and the nuclear magnetic resonance method.

Surface Chemistry **(25 marks) 20 hrs.**

A) Adsorption

Surface tension, capillary action, pressure difference across curved surface (Laplace equation), vapour pressure of droplets (Kelvin equation), Gibbs adsorption isotherm, estimation of surface area (BET equation), surface films on liquids (Electro-kinetic phenomenon), catalytic activity at surfaces.

B) Macromolecules

Polymer - definition, types of polymers, electrically conducting, fire resistant, liquid crystal polymers, kinetics of polymerization, mechanism of polymerization. Molecular mass, number and mass average molecular mass, molecular mass determination (Osmometry, viscometry, diffusion and light scattering

methods). Sedimentation, chain configuration of macromolecules, calculation of average dimensions of various chain structures.

Electrochemistry **(25 marks) 20hrs.**

Electrochemistry of solutions. Debye-Huckel-Onsager treatment and its extension, ion solvent interactions. Debye-Huckel-Jerum mode. Thermodynamics of electrified interface equations. Derivation of electrocapillarity, Lippmann equations (surface excess), methods of determination. Structure of electrified interfaces. Guoy-Chapman, Stern, Graham-Devnathan-Mottwatts, Tobin, Bockris, Devnathan models, Overpotentials, exchange current density, derivation of Butler-Volmer equation, Tafel plot. Debye-Huckel theory for activity coefficient of electrolytic solutions; determination of activity and activity coefficients; ionic strength.

M.Sc (Part I
(Semester II) (Paper 10)
Spectroscopy (80 marks)

Unit-1 :

Microwave spectroscopy **(10 marks) 03hrs.**

Classification of molecules, rigid rotor model, effect of isotopic substitution on the transition frequencies, intensities, non-rigid rotor. Stark effect, nuclear and electronic spin interaction and effect of external field. Applications.

Vibrationai Spectroscopy **(15 marks) 12 hrs.**

A) Infrared spectroscopy

Review of-linear harmonic oscillator, vibrational energies of diatomic molecules, zero point energy, force constant and bond strengths; anharmonicity, Morse potential energy diagram, vibration-rotation

spectroscopy, P,Q,R branches. Breakdown of Oppenheimer approximation; vibrations of polyatomic molecules. Selection rules, normal modes of vibration, group frequencies, overtones, hot bands, factors affecting the band positions and intensities, far IR region, metal-ligand vibrations, normal co-ordinate analysis.

B) Raman Spectroscopy

Classical and quantum theories of Raman effect. Pure rotational, vibrational and vibrational-rotational Raman spectra, selection rules, mutual exclusion principle. Resonance Raman spectroscopy, coherent Anti Stokes Raman spectroscopy (CARS).

Electronic Spectroscopy **(15 marks) 12hrs.**

A) Atomic Spectroscopy

Energies of atomic orbitals, vector representation of momenta and vector coupling, spectra of hydrogen atom and alkali metal atoms.

B) Molecular spectroscopy

Energy levels, molecular orbitals, vibronic transitions, vibrational progressions and geometry of the excited states, Franck-Condon principle, electronic spectra of polyatomic molecules. Emission spectra; radiative and non-radiative decay, Internal conversion, spectra of transition metal complexes, charge-transfer spectra.

Unit 2 :

Nulear magnetic resonance spectroscopy

(15 marks) 12 hrs.

Nuclear spin, nuclear resonance, saturation, shielding of magnetic nuclei, chemical shift and its measurements, fractors influencing chemical shift, deshielding, spin-spin interactions, factors influencing coupling constant 'J'.

Classification (ABX, AMX, ABC, A_2B_2), spin decoupling; basic ideas about instrument, NMR studies of nuclei other than proton-^{13}C, ^{10}F and ^{31}P, FT NMR, advantages of FT NMR, use of NMR in medical diagnostics.

Electronic spin resonance spectroscopy

(10 marks) 08 hrs.

Basic principles, zero field splitting and Kramer's degeneracy, factors affecting the 'g' value. Isotropic and anisotropic hyperfine coupling constants, spin Hamiltonian, spin densities and McConnell relationship, measurement techniques, applications.

X-ray diffraction **(15 marks) 12 hrs.**

Bragg condition. Miller indices, Laue method, Bragg method, Debye-Scherrer method of X-ray structural analysis of crystals, index reflections, identification of unit cells from systematic absences in diffraction pattern. Structure of simple lattices and X-ray intensities, structure factot and its relation to intensity and electron density, phase problem. Description of the procedure for an X-ray structure, analysis, absolute configuration of molecules, Ramchandran diagram.

(M.Sc Part I)
Semester II) (Paper 11)
Practical Inorganic Chemistry

Time : 6 hrs. **Full marks : 100**
(40+40+NB-10+V.V. 10)

A) Cent percent quantitative analysis of cement

B) Qualitative analysis of :

a) Haematite by $KMnO_4$ and $K_2CR_2O_7$

b) Brass

C) Estimation of the following :

a) Magnesium by EDTA methods (volumetrically)

b) Nickel by Dimethylglyoxime (Gravimetrically)

D) Preparation of the following metal complexes

a) Hexamine cobaltic chloride

b) Sodium Nitroprusside

c) Potassium trioxalato chromate

d) $K_3[FeC_2O_4)_3]$

e) Ni $(dimg)_2$

(M.Sc Part I)
(Semester II) (Paper 12)
Environmental Chemistry and Biochemistry Practical

Time - 6 hrs. **Full marks : 100**

Unit 1:

Environmental Chemistry (Practical) **(50 marks)**
(30+NB 5+W 15)

A) Determination of OD, BOD and COD of water

B) Determination of soil pollutants

C) Estimation of air pollutants

Unit 2 :

Biochemistry (Practical) **(50 marks)**
(30+NB 5+W 15)

A) Qualitative and quantitative estimation of protein

B) Qualitative and quantitative estimation of carbohydrate

C) Estimation of enzyme activity

M.Sc Part II

Course Details - M.Sc. (Part II)

(M-Sc Part II
(Semester III Paper 13)
Application of Specrtoscopv in inorganic chemistry
(80 marks)

Unit I:

Vibrational Spectroscopy **(15 marks) 05 hrs.**

Symmetry and shapes of AB2, Abs, AB4, ABs and Abe, mode of bonding of ambidentate ligands, ethyienediamine and diketonato complexes/application of resonance Raman Spectroscopy particularly for the study of active sites of metalloproteins.

Electron Spin Resonance Spectroscopv

(25 marks) OS

Hyperfine coupling, spin polarization for atoms and transition metal ions, spin-orbit coupling and significance of g-tensors, application to transition metal complexes (having one unpaired electron) including biological systems and to inorganic free radicals such as PFLt, ¥'2 and [BHa]".

Unit II:

Nuclear Magnetic Resonance of paramagnetic substances in solution (15 marks) 07 hrs.

The contact and pseudo contact shirts, factors affecting nuclear relaxation; some applications including biochemical systems, an oven/lei of NMR of metal nuclei with emphasis on 195_{Pt} and 119_{Sn} NMR.

Mossbauer Spectroscopv **(15 marks) 06 hrs**

Basic principles, spectral parameters and spectrum display. Applicatioi of the technique of the studies of (1) bonding and structures of Fe^{+2} anc Fe^{+2} compounds including those of intermediate spin, (2) Sn^{2+} and and Sn^{4+} compounds - nature of M-L bond, co-ordination number, structure anc (3) detection of oxidation state and inequivalent MB atoms.

(M.Sc Part II)
(Semester III Paper 14) Bio-chemistrv
(Bio-inorganic) (80 marks)

Unit I:

Metal ions in biological systems **(15 marks) 5 hrs.**

Essential and trace metals

Na^+/K^+ pump

Role of metal ions in biological processes

Bio-energetics and ATP cycle **(15 marks) 6 hrs.**

DNA polymerization, glucose storage, metal complexes in transmission of energy, chlorophylls, photo system I and photosystem II in cleavage of water. Model systems.

Unit II:

Transport and storage of Dioxygen (25 marks) 8hrs.

Heme proteins and oxygen uptake, structure and function of haemoglobin, myoglobin, hemocyanins and hemerythrin, model synthetic complexes of iron, cobalt and copper.

Electron transfer in Biology **(15 marks) 6 hrs.**

Structure and function of matalloproteins in electron transport processes- cytochromes and ion-sulphur proteins, synthetic models.

Nitrogenase **(10 marks) 5 hrs.**

Biological nitrogen fixation, molybdenum nitrogenase, spectroscopic and other evidence nitrogenases model system.

(M.Sc Part II)
(Semester III Paper 15)
Environmental Chemistry (80 marks)

Environment **(10 marks) 8 hrs.**

Introduction. Composition of atmosphere, vertical temperature, heat budget of the earth atmospheric system, vertical stability atmosphere. Biogeochemical cycles of C, N, P, S and 0. Biodistribution of elements.

Hydrosphere **(15 marks) 12 hrs.**

Chemical composition of water bodies - lakes, streams, rivers and wet lands. Hydrological cycle. Aquatic pollution-inorganic, organic, pesticide, agricultural, industrial and sewage, detergents, oil spills and oil pollutants. Water quality parameters - dissolved oxygen, biochemical oxygen

demand, solids, metals, content of chloride, sulphate, phosphate, nitrate and micro-organisms. Water quality standards. Analytical methods for measuring BOD, DO, COD, F, Oils/metals (As, Cd, Cr, Hg, Pb, Se), residual chloride and chlorine demand. Purification and treatment of water.

Soils **(5 marks) 6 hrs.**

Composition, micro and macro nutrients. Pollution - fertilizers, pesticides, plastics and metals. Waste treatment.

Unit II:

Atmosphere **(10 marks) 8 hrs.**

Chemical composition of atmosphere - particles, ions and radicals and their formation. Chemical and photochemical reactions in atmosphere, smog formation, oxides of N, C, S, O and their effect. Pollution by chemicals, petroleum, minerals, chlorofluoro-hydrocarbons. Green house effect, acid brain, air pollution, controls and their chemistry. Analytical methods for measuring air pollutants. Continuous monitoring instruments.

Industrial Pollution **(20 marks) 12 hrs.**

Cement, sugar, distillery, drug, paper and pulp, thermal power plants, nuclear power plants, metallurgy. Polumers, drugs. Radionuclide analysis. Disposal of wastes and their management.

Environmental Toxicology **(20 marks) 14 hrs.**

Chemical solutions to environmental problems, biodegrability, principles of decomposition, better industrial processes. Bhopal gas tragedy, Chernobyl, Three mile island, Sewozo and Minamata disasters.

(M.Sc Part II)
(Semester III Paper 16)
Analytical Chemistry (80 marks)

A) **Chromatography** (15 marks) 12 hrs.

Paper

TLC,

Liquid

GLC

HPLC

Colun

B) **Electrophoresis** (10 marks) 5 hrs.

Paper, etc., reverse osmosis

C) **Centrifuation** (10 marks) 5 hrs.

for biomolecules Ultra, vacuum.

D) **Spectroscopic** (15 marks) 12 hrs.

UV-vis

IR & FTIR

NMR [solid/liquid]

E) **Marometer** (10 marks) 5 hrs.

a) constant pressure

b) constant volume
Dialysis

F) **Thermal analysis** (20 marks) 16 hrs.

Thermogravimetric	TGA
Theranalysis	TMA
Differe	DTA
Glass Transition Temperature	Tg

(M.Sc Part II
(Semester III Paper 17)
Practical Organic Chemistry

Time - 6 hrs. Full marks : 100
(30+30+20+NB-5+V.V. 15)

A) **Organic Qualitative**

Identification of organic compounds containing not more than two functional groups using chemical analysis.

B) Preparation of organic compounds using methods not involving more than two steps.

Some of the experiments listed below :

a) Preparation of methyl orange

b) Preparation of o-chlorobenzoic acid

c) Preparation of Diphenic acid

d) Preparation of Martius yellow

e) Preparation of 2:4:6 tribromo phenol from aniline

f) Preparation of p-nitro aniline from acetanilide

g) Preparation of sulphanilic acid from aniline

h) Preparation of cinnamic acid from benzaldehyde

C) **Estimation of**

a) Glucose

b) Nitrogen from Kjeldahl's method

c) Carbonyl group using 2:4 dinitrophenyl hydrazine

(M.Sc PartII)
(Semester III Paper 18)
Practical Analytical Chemistry

Time - 6 hrs.
Full marks : 100
(40+40+NB 10+V.V.10)

A) **Chromatography**

TLC

Paper

B) **Electrophoresis**

C) **Dialysis**

D) **UV-vis**

E) **Calorimetric estimation of glucose- DNS**

F) **pH**

G) **Conductometric titration**

H) **Potentiometric titration**

(M.Sc Part II)
(Semester IV Paper 19)
Special Paper (80 marks)
(Eight Questions are to be set)
(Five Questions are to be answered)

Inorganic Chemistry

Time - 3 hrs.
Full marks - 80

Alkyls and aryls of transition metals (1Q) 5 hrs.

Types, routes of synthesis, stability and decomposition pathways, organocopper in organic synthesis.

Compounds of transition metal-carbon multiple bonds (2Q) 12 hrs.

Alkylidenes, alkylidynes, low valent carbenes and carfynes-synthesis, nature of bond, structural characteristics, nucleophilic and electrophilic reactions on the ligands, role in organic synthesis.

Transition metals re-complexes (2Q) 18 Hrs.

Transition metal n-complexes with unsaturated organic molecules, alkenes, alkynes, alkyl, diene,dienyl, arene and trienyl complexes, preparations, properties, nature of bonding and structural features. Important reactions relating to nucleophilic and electrophilic attack on ligands and to organic synthesis.

Homogeneous catalysis (2Q) 14 Hrs.

Stoichiometric reactions for catalysis, homogeneous catalytic hydrogenation, Zeigler-Natta polymerization of olefins, catalytic reactions involving carbon monoxide such as hydrocarbonylation of olefins (oxo reaction), oxopalladation reactions, activation of C-H bond.

Fluxional Organometallic compounds (1Q) 8 hrs.

Fluxionality, and dynamic equilibria in compounds such as η^3- olefin, $l1^3$ atlyl and dienyl complexes.

Organic Chemistry (Special)

Time - 3 hrs. **Full marks - 80**

Terpenoids and Cartenoids (1Q) 15 hrs.

Classification, nomenclature, occurrence, isolation, general methods of structure determination, isoprene rule.

Structure determination, stereochemistry, biosynthesis and synthesis of the following representative molecules: Citral, α-Terpeneol, Zingiberene, Santonin.

Alkaloids (1Q) 15 hrs.

Definition, nomenclature and physiological action, occurrence, isolation, general methods of structure elucidation, degradation, classification based on nitrogen heterocyclic ring, role of alkaloids in plants. Structure, stereochemistry, synthesis and biosynthesis of the following : Atropine, Quinine and Morphine.

Steroids (1Q) 15 hrs.

Occurrence, nomenclature, and basic skeleton, Diel's hydrocarbon and stereochemistry, isolation, structure determination and synthesis of Cholestrol. Andosterone/Testosterone, Estrone, Progestrone, Aldosterone. Biosynthesis of steroids

Proteins and lipids (1Q) 15 hrs.

Classification of naturally occurring peptides, sequence determination, chemical and enzymatic reactions. Peptide synthesis, protection and deprotection, solid phase

synthesis, chemistry of oxytocin and valinomycin. Classifl-cation of fatty acids and lipids, synthesis of phospholipids and glycolipids.

Principles of reactivity **(1Q) 5 hrs.**

Mechanistic signlficance of entropy, enthalpy and Gibbs free energy, Arrhenius equation, transition state theory. Uses of activation parameters, Hammond's postulate. Bell-Evans-Polanyi principle. Potential energy surface model. Marcus theory of electron transfer. Reactivity and selectivity principles.

Kinetic isotope effect **(1Q) 4 hrs.**

Theory of isotope effects, primary and secondary kinetic isotope effects. Heavy atom isotope effects, Tunneling effect. Solvent effects.

Structural effects on Reactivity **(1Q) 6 hrs.**

Linear free energy relationships (LFER). The .Hammett equation., substituent constants, theories of substituent effects. Interpretation of o-values. Reaction constant p. Devlations from Hammett equation. Dual-parameter correlations, inductive substituent constant. TheTaft model, ol and o R-scale.

Solvation and Solvent Effects **(1Q) 6 hrs.**

Qualitative understanding of solvent-solute effects on reactivity. Thermodynamic measure of salvation. Effects of salvation on reaction rates and equilibria. Various empirical indexes of solvation based on physlcal properties, solvent-sensetive reaction rates, solvent effects from the curve-crossing mode.

Physical Chemistry f Special)

Time : 3 hrs. **Full Marks : 80**

A) **Diffraction of X-rays by crystals** - Debye Scherrer method, indexing powder pattern for cubic and

tetragonal crystals, rotating crystal method, Fourier transform and reciprocal lattices, Bragg equation in reciprocal lattice, neutron diffraction. **(1Q) 10 hrs.**

B) **Metallic bonds** - free electron theory, band theory, Fermi level, Brillouin zone, wave function for electrons In solids, metallic conductors, insulator, semi conductors (intrinsic and extrinsic) , properties of junctions. **(1Q) 10 hrs.**

C) **Super conductivity** - meissner effect, microscopic theory of 25

Physical Chemistry (Special)

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C) **Super conductivity** - meissner effect, microscopic theory of super conductivity, conventinal organic and high temp, super conductors, fullerences, applications of superconductors. Transformatin in crystals - thermo dynamics of transformation. **(1Q) 10 hrs.**

D) **Specific heat of solids** - classical theory, quntum theory of specific heats - Eastein **(1Q) 10 hrs.**

E) Polymer solutin, thermodynamics of polymer solutions, molar mass and molar mass distributin, methods of measuring molar masses, micelle formation and hydrophobic interaction.

F) Electrically conducting polymers, electrochemical polymerizatin, band structure of polymers, mechanism of conducin in polymers, doping of polymers, application of conduction polymers.

G) Polymer liquid crystal nematic, cholesteric and smectic phases, liquid crystalline order of the main chain and of the side groups in polymers, synthesis nd properties of polymer liquid crystals, liquid crystalline order in boiological materials.

H) **Surface chemistry** - Surface films, BEt isotherm for multilayers and its devrivation, kinetics of surface processes, unimolecular and biomolecular surface reactions, electrocapillarity, electrokinetic effects, statistical mechanics of adsorption. **(1Q) 10 hrs.**

(M. Sc. Part II)
(Semester IV Paper 20)
Special Paper (80 marks)

Time - 3 hrs. Full Marks - 80

Inorgamoc Chemistry
(SPecial)

Metal Storage transport and biomineralization **(1Q) 6 hrs.**

Ferritin, transferritin and siderophores.

Calcium in Biology **(1Q) 6 hrs.**

Calcium in living cells, transport and regulation, molecular aspects of intramolecular processes, extra cellular binding proteins.

Metalloenzymes **(2Q) 20 hrs.**

Zinc enzymes - Carboxypeptidase and carbonic Anhydrase. Iron enzymes - catalase, perxidase and cytochrome P-450. Copper enzymes - superoxide dismutase. Molybdenum oxatransferrase enzyme - xanthine oxidase. Co-enzyme vitamin B_{12}.

Metal - Nuclei acid interactions **(1Q) 6 hrs.**

Metal deficiency and disease, toxic effects of metals, metals used for diagnosis and chemotheraphy with particular refernce to anti-cancer drugs.

Supramolecular Chemistry **(2Q) 18 hrs.**

Concepst and language.

(a) Molecular recognization : molecular receptors for different types of molecules including arisonic substrates, design and synthesis of coreceptor molecules and multiple recognition.

(b) Supramolecular reactivity and catalysis.

(c) Transport processes and carrier design

(d) Supramolecular device. Supramolecular photochemistry, Supramolecular electronic, ionic and switching devices.

Some examples of self-assembly in Supramolecular Chemistry.

Organic Chemistry (Special)

Time - 3 hrs. **Full Mrks - 80**

Synthetic Drugs

(a) Nimesulide

(b) Ibuprofen

(c) Isonicotinic hydrazide

(d) dytide

(e) Methotrexate

Structure determination and synthesis of Vit. A, B1, B2, B6, Vit. C and Vit. D. **(2Q) 15 hrs.**

Antibiotics **(1Q) 20 hrs.**

a) Tetracycline
b) Cesuroxime
c) Chloromycelin

General mechanism of drug action on lipid, carbohy drate and protein.

Steric and Conformatinoal Properties **(1Q) 6 hrs.**

Various thpes of steric strain and their influence on rectivity. Steric acceralation. Molecular measurements upon steric effects upon rates. Steric LFER. Conformational barrier to bond rotation - spectroscopic detection of individual conformers. Acyclic and monocyclic systems. rotation around partial double bonds. Winstein-Holness and Curtin-Hammett principle.

Nucleic Acid **(2Q) 20 hrs.**

Secondary, tertiary and quaternary structures of DNA and RNA, also synthesis of nucleosides and nucleotides.

Enolates **(1Q) 18 hrs.**

Thermodynamic versus kinetic enolates, enamines. Its application in carbon-carbon bond formation. application in chiral synthesis.

Physical Chemistry (Special)

Time - 3 hrs. **Full Marks - 80**

Potential Energy Surfaces

Mechanical of activation, potential energy surface for three atom reaction, potential energy curve for successive reactions, proportions of potential energy surfaces, interconversion of translational and vibratinal energies, combinatino of atoms, ortho-para conversion, activated state of three atom and four atom reactions, potential energy profile, reaction co-ordinate, transmission co-efficient, non-adiabatic reaction.

Kinetics of condensed phase reactions **(2Q) 20 hrs.**

Rate determining steps in diffusion control reactions and activation controlled reactions, Stokes-Einstein equation and dependence of rate constant on co-efficient of viscosity of medium, kinetics of ionic reactions in solution-electrostatic contribution to free energy in single and spherical models of activated complex, entropy of activation for ion-ion reactins

; kinetics of dipole-dipole reactin, ion-dipole reaction, dependence of rate constant on ionic strength and dielectric constant of medium, Bronsted-Bjerrum equation.'

Catalysis and Oscillation **(1Q) 20 hrs.**

Kinetics of catalytic reactinos, theory of acid-base catalysis, van'tHoff and Arrhenius complexes, progenetic and protophilic mechanisms, effect of salt on acid base catalysis, auto catalysis, non-competitive and competitive inhibitors, Bronsted catalysis law, rate of reaction and acidity functions, linear free energy relationship, Hammett equation, meaning of substituent constant and reaction constant in organic reactions, reactions in biological systems. Oscillating reactions, Lotka-Voltera model, B-Z reaction. The brus organator, bistability, Chemical chaos.

Study of fast rections **(1Q) 12 hrs.**

Photophysical chemistry - Flash photolysis, Relaxtion technique, nuclear magnetic reasonance method, molecular Beam and Shock-tube kinetics, flow method. Reactions of protons, electrons, metal ions.

Electrode Kinetics **(2Q) 18 hrs.**

Faradaic and non-faradaic current, rate law in Farads Process, current density, factors affecting electrode reaction, types of overvoltage, polarisatin, polarisation curves, electric potential, derjvatin of Nernst equation (i) on thermodynamic consideration and (ii) by kinetic approach Tafel plot. butler-volmer equatin, Nornst diffusion layer treatment, exchange current density, stoichiometric number, concept of rate determining steps, energy barriers for multistep reactions. Studies on electrode kinetics-polarographic analysis, rotating disc convectin method.

Electrode Deposition and Corrosion Processes **(1Q) 18 hrs.**

Electrocatalysis-electrocatalytic rate, electrocatalys in redox system. Total depositin current density, time variatin of the

overpotential, and rate determining step in electrode deposition. Total overpotential fo electrode deposition at steady state Hydrogen overvoltage, rate determining steps of the hydrogen evolutin reactin, determination of reaction order with respect to H+ ions in solution. Corrosion current, electronatin current and corrosion potentlal, elecronation reaction, corrosion and stability of metals.

(M. Sc. Part II)
Semester IV Paper 21)
Bio-Chemistry (80 marks)
(Bio Organic)

Unit 1 :

Enzymes and mechanism of enzyme action
(15 marks) 6 hrs.

Basic considerations. Proximity effects and molecular adaptation.

a) **Enzymes** **(15 marks) 6 hrs.**

Introduction and hostorical perspective, chemical and biological catalysis, remarkable properties of enzymes like catalytic power, specificity and regulation. Nomenclature and clssification, extraction and purification. Fischer's lock and key and Konstand's induced fit hypothesis, concept and identification of active site by the use of inhibitors. Affinity labelling and enzyme modification by site-directed mutagenesis enzyme kinetics. Michaelis-menten and Lineweaver-burk plots, reversible and irreversible inhibition.

b) **Mechanism of enzyme action** **(10 marks) 3 hrs.**

Transition-state theory, orientation and steric effect acid-base catalysis, covalent catalysis, strain or distortion. Example of some typical enzyme mechanism for chymotrypsin, ribonuclease, lysozyme and carboxypeptidase A.

Unit II :

Kinds of reactins catalysed by enzymes
(15 marks) 8 hrs.

Nucleophilic displacement on a phosphorus atom, multiple displacement reactions and the coupling of ATP cleavage to endergonic processes. Transfer of sulphate, addition and elimination reactions, enolic intermediates in isomerizatin reactions, p-cleavage and condensation, some isomerizatino and rearrangement reaction. Enzyme catalysed carboxylation and decarboxylation.

Co-Enzyme Chemistry **(15 marks) 14 hrs.**

Cofactor as derived from vitamins, coenzymes, prosthetic groups, apoenzymes. Structure and biological functions of coenzyme A, thiamine pyrophosphate, pyridoxal phosphate, NDA+, NADP^FMN, FAD, lipofc acid, vitamin 812. Mechanisms of reactins catalysed by me above cofactors.

Biotechnological applications of enzymes
(15 marks) 15 hrs.

Large-scale production and purficatin of enzymes, techniques and methods of immobilization of enzymes, effect of immobilization on enzyme activity, application of immobilized enzymes, use of enzymes in foods and drink industry- brewing and cheese-making, syrup from cornstrach, enzymes as targets for drug design. Clinical uses of enzymes, enzyme theraphy, enzymes and recombinatino DNA technology.

(M. Sc Part II)
(Semseter IV Paper 22)
Application of spectroscopy in Organic Chemistry
(80 marks)

Unit 1:

A) Ultraviolet and visible Spectroscopy
(10 marks) 5hrs.

Various electronic transition (185-800nm), Beer-

Lambert law, effect of solvent on electronic transitlon ultra voilet bands for carbonyl compounds, unsaturated carbonyl compounds, dienes, conjugated polyenes. Fieser-Woodward rules for conjugated dienses and carbonyl compounds, ultra voilet spectra of aromatlc and heterocyclic compounds.

B) Infrared spectroscopy (15 marks) 5hrs.

Instrumentatlon and sample handling. Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenol and amines. Detailed study of vlbrational freqnencies of carbonyl compounds (ketones, aldehyde, esters, amides, acids, lactones, lactams and conjugated carbonyl compounds). Effect of H-bonding and solvent effect on vibrational freqnencies, overtones, combination bands and Fermi resonance. FT-IR. IR of gaseous, solids and polymetrlc material.

Unit II :

A) Carbon-13 NMR Spectroscopy (15 marks) 5 hrs.

General considerations, chemical shlft (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbon), coupllng constants. Two dimenslon NMR spectroscopy - COSY, NOESY, DEPT, INEPT, APT and INADEQUATE techniques.

B) Mass spectrometry (20 marks) 12 hrs.

Introductlon, ion production - El, Cl, FD and FAB, factors ffecting ragmentatlon, ion analysls, ion abundance. Mass spectral fragmenttin of organic compounds, common functinoal groups, moleculr ion peak, metastable peak, McLafferty rerrangement. Nitrogen rule, high resolutlon mass, spectrometry. Examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

(M. Sc. Part II)
Semester IV Paper 23)
Practical : Special
(Inorganic Chemistry Practical)

Time : 12 hrs. **Full Marks : 100**

Quantitative Analysis

(I) Analysis of alloys (brass)

(ii) Calorimetric estimation of cations/anlons.

Separatin Techniques

Chromatography Separation

(i) Zn-Mg

Preparation of simple inorganic complexes, their purification, molecular weight determination and elucidatin of the avallable physical methods.

(a) Preparation of Cobalt (II) complexes

(I) $[Co(NH_3)_5Cl]\ Cl_2$

(b) (i) Purlfication of inorganic complexes using techniques such as crystallization, volatisation.

(ii) Tests for purity - M:P., TLC, Metal analysis etc.

Flame Photometric Determinations

Sodium and Potassium when present together

Determinatlon of

Manganese / Chromium / Vanadium in steel sample by spectro-photometric method

Organic Chemistry Practical (Special)

time : 12 hrs. **Full Marks : 100**

Organic synthesis and extraction of organic comounds from natural sources

(a) Extractin of caffine frmo tea leaves

(b) Isolation of casein from milk (try some typical colour reactions of proteins).

(c) Isolation of lactose from milk (check purity of sugar by TLC and PC and calculate RF values).

(d) Isolation of nicotine dipicrate from tabacco.

(e) Preparation of indigo from anthranilic acid

Quantitative Analysis

(a) Estimation of carbonyl group by using 2, 4-dinitrophenyl-hydrazine.

(b) To estimate nitrogen in the given sample by Kjeldahl method.

(c) To determine the percentage or number of hydroxyl groups in the given sample by the acetylation method.

(d) To determine the iodine number of the given fat or oil sample.

Physical Chemistry Practical (Special)

Time : 12 Hrs. Full Marks : 100

Conductometry

(a) To determine the solubility and solubility product of a sparingly soluble salt.

(b) to determine the rate constant of saponification of an ester by NaOH.

Potentiometry

(a) To determine the solubility and solubility product of AgCl in water.

(b) To determine the EO of Zn/Zn^{++}, Cu/Cu^{++} electrodes.

Polarimetry

(a) To analyse a mixture of glucose and sucrose

Group - B

Chemical Kinetics

(a) To determine the rate constant of the reaction between $K_2S_2O_8$ and KI at two different temo. And hence to determine the energy of activation of the reaction.

Thermochemistry

(a) Determination of basicity of a polybasic acid,

(b) Determination of heat of disniacement of Cu by Zn from Cu_2+ sait solution.

Distribution Law

(a) Determination of equiiibrium constant for the reaction $KI+I_2 = KI_3$.

Thermodanamics and Surface Chemistry

(a) To study the adsorption of acetic acid on charcoal.

Viscosity and Surface Tension.

(a) To determine the parachor of - CH, C and H.

(M. Sc. Part II)
(Semester IV Paper 24)
Project Work

Project - 75, Presentation 25) **Full Marks : 100**

The paper wiii consist of

(a) Fieid work/Lab work related to the project.

(b) Preparation of desertation based on the work undertaken.

N.B.: The students wiii select topic for the project work in consultation with a teacher of the Department.

Topics

Project work related to the following Industriai/Socially relevant topics may be given to th students of M. Sc II in Paper - XIV.

(a) Environmental study such as (i) Analysis of water, soil, air etc.

(b) Industrial goods analysis such as

i) Analysis of minerals available in Jharkhand state

ii) Analysis of minerals available in Jharkhand state

iii) Synthesis of useful commercial products based on raw materials available in Jharkhand state such as Lac, Limestone etc.

iv) Isolation of Constituents of medicinal plants available in Jharkhand state

Each student hs to submit two copies will be submitted in the Department of Chemistry, JWC for evaluation (Seven days before the seminar).

N.B. : The seminar (read the syllabus) will be held in the Department of Chemistry, JWC.