RANCHI WOMEN'S COLLEGE

RANCHI

(Autonomous College)

Constituent Unit

Of

Ranchi University,Ranchi

Syllabus of Chemistry for PG

Under Choice Based Credit System(CBCS)

DEPARTMENT OF CHEMISTRY

Meeting of Board of Studies

07.04.2021

A meeting of Board of Studies of Chemistry was held in the department of Chemistry Ranchi Women's College on 07.04.2021 at 11:30 AM

MEMBERS OF BOARD OF STUDIES

1. Chair person:- Dr. Shobhana Sharan (Head of Deptt. Chemistry)
2. Experts:-
   - i. Dr. K.N. Thakur (Retd.) Department of Chemistry, Ranchi College, Ranchi
   - ii. Dr. Nand ~~Kishor~~ Keshri, P.G. Head, Department of Chemistry, R.U. Ranchi
   - iii. Dr. H.O. Pandey, Associate Professor, Department of Chemistry, R.U. Ranchi
3. Members of Committee:-
   - i. Dr. Neeta Sinha
   - ii. Dr. Neelam
   - iii. Dr. Reena Bhadani
   - iv. Ms. Pratibha Mahto
   - v. Ms. Juhi Baranwal
   - vi. Dr. Preeti Sinha
4. Ms. Komal Kumari, PG(2019-21)
5. Ms Shweta Kumari, UG(2018-21)

Agenda of Meeting:

To review the syllabus of CBCS course of UG / PG Chemistry and to make any changes if required.

Resolution

1. Change in project of PG Semester IV
2. Inclusion of Pericyclic reaction in PG Sem III and removal of terpenoids and caretenoids
3. Inclusion of heterocyclic compounds 5-membered and 6-membered with one hetero atom, omitting dyes.
4. Minor changes in Honors practical of Physical Chemistry in UG semesters.
5. Removal of certain irrelevant topics in Inorganic Chemistry of GE of UG courses.

Member Secretary
Academic Council
Ranchi Women's College

CHAIRPERSON
ACADEMIC COUNCIL
RANCHI WOMEN'S COLLEGE

Semesterwise Distribution of Course

Chemistry
M.Sc. Semester-1
FC – Compulsory (FC-1)

Full Marks: 70+30
Time : 03 Hours

Total Lecturer : 70 Hours

Instruction to Question Setter:

Mid Semester Examination (MSE):
*There will be **two** groups of questions in written examinations of 20 marks. **Group A is compulsory** and will contain five questions of **very short answer type** consisting of 1 mark each. **Group B will contain descriptive type five** questions of five marks each, out of which any three are to be answered.*

End Semester Examination (ESE):
*There will be **two** groups of questions. **Group A is compulsory** and will contain two questions. **Question No.1 will be very short answer type** consisting of five questions of 1 mark each. **Question No.2 will be short answer type** of 5 marks. **Group B will contain descriptive type six** questions of fifteen marks each, out of which any four are to be answered.*

Note: *There may be subdivisions in each question asked in Theory Examinations*
*The Mid Semester Examination shall have three components. (a) Two Semester Internal Assessment Test (SIA) of 20 Marks each, (b) Class Attendance Score (CAS) of 5 marks and (c) Class Performance Score (CPS) of 5 marks. "**Better of Two**" shall be applicable for computation of marks for SIA.*

(Attendance Upto75%, 1mark; 75<Attd.<80, 2 marks;80<Attd.<85, 3 marks;85<Attd.<90, 4 marks;90<Attd, 5 marks).

I Stereochemistry and Bonding in Main Group Compounds **09 Hrs**

VSEPR, Walsh diagrams (tri-atomic molecules of type AH_2), dp-pp bonds, Bent rule and energetic of hybridization, some simple reactions of covalently bonded molecules, Atomic Inversion , Berry Pseudorotation.

II Nature of Bonding in Organic Molecules **12 Hrs**

Delocalized chemical bonding-conjugation, cross conjugation, resonance, hyper conjugation, bonding in fullerenes, tautomerism.

Aromaticity in benzenoid and non-benzenoid compounds, alternant and non-alternant hydrocarbons, Huckel's rule, energy level of 7-molecular orbitals, annulenes, antiaromaticity, tV-aromaticity, homo-aromaticity, PMO approach.

Bonds weaker than covalent- addition compounds, crown ether complexes and cryptands, inclusion compounds, cyclodextrins, catenanes and rotaxanes.

III Stereochemistry **16 Hrs**

Conformational analysis of cycloalkanes, decalins, effect of conformation on reactivity, conformation of sugars, steric strain due to unavoidable crowding.

Elements of symmetry, chirality, molecules with more 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.

IV Introduction to Exact Quantum Mechanical Results 09 Hrs

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.

V Unifying Principles 12 Hrs

Electromagnetic radiation, interaction of electromagnetic radiation with matter-absorption, emission, transmission, reflection, refraction, dispersion, polarisation and scattering. Uncertainty 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.

VI Metal-Ligand Equilibria in Solution 12 Hrs

Step wise and overall formation constants and their interaction, trends 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 formation constants by pH-metry and spectrophotometry.

Books Suggested

1. Inorganic Chemistry, J.E. Huhey, Harpes & Row.
2. Advanced Organic Chemistry-Reactions, Mechanism and Structure, Jerry March, John Wiley.
3. Introduction to Quantum Chemistry, A.K. Chandra, Tata McGraw Hill.
4. Quantum Chemistry, Ira N. Levine, Prentice Hall.

5. Chemical Applications of Group Theory, F. A. Cotton.
6. Physical' Methods in Chemistry, R.S. Drago, Saunders College.
7. Introduction to Molecular Spectroseopy, Q.M. Barrow, McCraw Hill.

Chemistry
M.Sc. Semester-1
Core Course – 1 (CC-1)

Full Marks: 70+30
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(Attendance Upto75%, 1mark; 75<Attd.<80, 2 marks;80<Attd.<85, 3 marks;85<Attd.<90, 4 marks;90<Attd, 5 marks).

I Reaction Mechanism of Transition Metal Complexes — 25 Hrs

Energy profile of a reaction, reactivity of metal complexes, inert and labile complexes, kinetic application of valence bond and crystal field theories, kinetics of octahedral substitution, acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, direct and indirect evidences in favour of conjugate mechanism, anation reactions, reactions without metal ligand bond cleavage. Substitution reactions in square planar complexes, the trans effect, mechanism of the substitution reaction. Redox reactions, electron transfer reactions, mechanism of one electron transfer reactions, outer-sphere type reactions, cross reactions and Marcus-Hush theory, inner sphere type reactions

II Metal π-Complexes — 16 Hrs

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

III Metal-Ligand Bonding — 08 Hrs

Limitation of crystal field theory, molecular orbital theory, octahedral, tetrahedral and square planar complexes, p-bonding and molecular orbital theory.

IV Electronic Spectra and Magnetic Properties of Transition Metal Complexes 15 Hrs

Spectroscopic ground states, correlation, Orgel and Tanabe-Sugano diagrams for transition metal complexes (d^1-d^9 states), calculations of Dq, B and b parameters, charge transfer spectra, spectroscopic method of assignment of absolute configuration in optically active metal chelates and their stereochemical information, anomalous magnetic moments, magnetic exchange coupling and spin crossover.

V Metal Clusters 06 Hrs

Higher boranes, carboranes, metalloboranes and metallocarboranes. Metal carbonyl and halide clusters, compounds with metal-metal multiple bonds.

Books Suggested

1. Advanced Inorganic Chemistry, F.A. Cotton and Wilkinson, John Wiley.
2. Inorganic Chemistry, J.E. Huhey, Harpes & Row;
3. Chemisiry ol the Elements, N.N. Greenwood and A. Earnshow, Pergamon.
4. Inorganic Electron ioSpeci roscopy, A. B. P. Leve r, Elsevier.
5. Magnetochemistry, R.L. Cariin, Springer Vertag,
6. Comprehensive Coordination Chemistry eds., Q. Wilkinson, R.D. Gillars and J.A. McCleverty, Pergamon.

Chemistry
M.Sc. Semester-I
Core Course – 2 (CC-2)

Full Marks: 70+30
Time : 03 Hours

Total Lecturer : 70 Hours

Instruction to Question Setter:

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1 Reaction Mechanism: Structure and Reactivity 20 Hrs

Types of mechanisms, types of reactions, thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond's postulate, Curtin-Hammett principle. Potential

energy diagrams, transition states and intermediates, methods of determining mechanisms, isotope effects. Hard and soft acids and bases.
Generation, structure, stability and reactivity of carbocations, carbanions, free radicals, carbenes and nitrenes.
Effect of structure on reactivity resonance and field effects, steric effect, quantitative treatment. The Hammett equation and linear free energy relationship, substituent and reaction constants. Taft equation.

II Aliphatic Nucleophilic Substitution **20 Hrs**

The S_N2, S_N1, mixed S_N1 and S_N2 and SET mechanisms.
The neighbouring group mechanism, neighbouring group participation by R and a bonds, anchimeric assistance.

Classical and nonclassical carbocations, phenonium ions, norbornyl system, common carbocation rearrangements. Application of NMR spectroscopy in the detection of carbocations.

The SNi mechanism. Nucleophilic substitution at an allylic, aliphatic 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.

III Aliphatic Electrophilic Substitution **07 Hrs**

Bimolecular mechanisms- S_E2 and S_Ei. The $_{SO}$ mechanism, electrophilic substitution accompanied by double bond shifts.
Effect of substrates, leaving group and the solvent polarity on the reactivity.

IV Aromatic Electrophilic Substitution **08 Hrs**

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 substrates and electrophiles. Diazonium coupling, Vilsmeir reaction, Gattermann-Koch reaction.

V Aromatic Nucleophilic 'Substitution **03 Hrs**

The S_NAr, $_{SO}$, benzyne and $_{SRO}$ mechanisms. Reactivity - effect of substrate structure, leaving group and attacking nucleophile. The von Richter, Sommelet-Hauser, and Smiles rearrangements.

VI Free Radical Reactions **12 Hrs**

Types of free radical reactions, free radical substitution mechanism, mechanism at an aromatic substrate, neighbouring group assistance. Reactivity for aliphatic and aromatic substrates at a bridgehead. Reactvity in the attacking radicals. The effect of solvents on reactivity. Allylic halogenation (NBS), oxidation of aldehydes to carboxylic acids, auto-

oxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts. Sandmeyer reaction. Free radical rearrangement. Hunsdiecker reaction.

Books Suggested

1. Advanced Organic Chemistry-Reactions, Mechanism and Structure, Jerry March, John Wiley.
2. Advanced Organic Chemistry, F. A. Carey and R. J. Sundberg, Plenum.
3. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.
4. Structure and Mechanism in Organic Chemistry, C. K. Ingold, Cornell University Press.
5. Organic Chemistry, R. T. Morrison and R. N. Boyd, Prentice-Hall.
6. Modern Organic Reactions, H. 0. House, Benjamin.
7. Principles of Organic Synthesis, R. 0. C. Norman and J. M. Coxon, Blackle Academic & Professional.
8. Pericyclic Reactions, S. M. Mukherji, Macmillan, India.
9. Reaction Mechanism in Organic Chemistry, S. M. Mukherji and S. P. Singh, Macmillan.
10. Stereochemistry of Organic Compounds, D. Nasipuri, New Age international.
11. Stereochemistry of Organic Compounds, P.S. Kalsi, New Age International.

Chemistry
M.Sc. Semester-1
Core Course (P) – 3 [CC(P)-3]

Full Marks: 100
Time : 06 Hrs

1. Cent per cent quantitative Analysis of Cement
3. Estimation of the following:
   - (a) Magnesium by E.D.T.A. Methods (Volumetrically)
   - (b) Zinc by potassium ferrocyanide (Volumetrically)
   - (c) Nickel by Dimethylglyoxime (Gravimetrically)
   - (d) Managnese in steel by sodium bismuthate method.

4 Organic Qualitative

Identification of organic compounds containing one functional group using Chemical Analysis

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

Some of the experiments listed below:

- (i) Preparation of methyl Orange
- (iv) Preparation of Martius yellow
- (vi) Preparation of p-nitro aniline from acetanilide
- (viii) Preparation of Cinnamic acid from Benzaldehyde

III Estimation of Glucose

Chemistry
M.Sc. Semester-II
Elective Course (SE) (EC-1)

Full Marks: 70+30
Time : 03 Hours

Total Lecturer : 70 Hours

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I Introduction to Computers and Computing — 10 Hrs

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 of programming. Algorithms and flow-charts.

II Computer Programming in C Language — 20 Hrs

Elements of the Computer Language Constants and variables and data types. Operators and Expressions, Arithmetical, Relational, Logical, Assignment, Increment and Decrement operators. Input and output statements. Branching statements such as (if-else, goto, switch) statements. Decision making and looping (while, for, do). Arrays (one dimensional and two dimensional arrays). Sorting of data in an array. Function (user defined functions).

III Programming in Chemistry — 25 Hrs

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

IV Use of Computer Programmes **15 Hrs**

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, ORIGIN, MATLAB.

Books Suggested

1 Comdex Computer Course kit (XP Edition), Vikas Gupta, Dreamtech, New Delhi
2. Fox Pro For DOS & Windows, R.K.Taxali, BPB Publication.
3. Programming in ANSIC, E. Balaguruswamy, Tata McGraw Hill
4. Computer for Chemist Bansal, Pragati Prakshan

OR

BIO-CHEMISTRY

GROUP-A

I **Metal Ions in Biological Systems** **03 Hrs**

Essential and trace metals. Na^+/K^+ Pump

Role of metals ions in biological processes,

II **Bioenergetics and ATP Cycle** **08 Hrs**

DNA polymerisation, glucose storage, metal complexes In transmission of energy; chlorophylls, photosystem I and photosystem II in cleavage of water. Model systems.

III **Transport and Storage of Dioxygen** **05 Hrs**

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

IV **Electron Transfer in Biology** **08 Hrs**

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

Nitrogenase **05 Hrs**

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

GROUP B

I **Enzymes and Mechanism of Enzyme Action** **02 Hrs**

Basic considerations. Proximity effects and molecular adaptation.

Enzymes **10 Hrs**

Introduction and historical perspective, chemical and biological catalysis, remarkable properties of enzymes like catalytic power, specificity and regulation. Nomenclature and classification, extraction and purification. Fischer's lock and key and Koshtand's induced fit hypothesis, concept and identification of active site by the use of inhibitors, affinity labeling and enzyme modification by site-directed mutagenesis. Enzyme kinetics, Michaelis-Menten and Lineweaver-Burk plots, reversible and irreversible Inhibition.

Mechanism of Enzyme Action **06 Hrs**

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

II **Kinds of Reactions Catalysed by Enzymes** **08 Hrs**

Nucleophilic displacement on a phosphorus atom, multiple displacement reactions and the coupling of ATP cleavage to endergonic processes. Addition and elimination reactions, enolic intermediates in isomerization reactions, p-cleavage and condensation, some isomerization and rearrangement reactions. Enzyme catalyzed carboxylation and decarboxylation.

III **Co-Enzyme Chemistry** **05 Hrs**

Cofactors as derived from vitamins, coenzymes, prosthetic groups, apoenzymes. Structure and biological functions of coenzyme A, thiamine pyrophosphate, pyridoxal phosphate, NAD^+, $NADP^+$ FMN, FAD, lipolc acid, vitamin B_{12}. Mechanisms of reactions catalyzed by the above cofactors.

IV Biotechnological Applications of Enzymes **10 Hrs**

Large-scale production and purification of enzymes, techniques and methods of immobilization of enzymes, effect of immobilization on enzyme activity, application of immobilized enzymes, use of enzymes in food and drink industry-brewing and cheese-making, syrups from corn starch, enzymes as targets for drug design. Clinical uses of enzymes, enzyme therapy, enzymes and recombinant DNA technology.

Books Suggested

1. Principles of Bioinorganic Chemistry, S.J. Lippard and J.M. Berg, University Science Books.
2. Bioinorganic Chemistry, I. Bertini, H.B. Gray, S.J. Lippard and J.S. Valentine, University Science Books.
3. Inorganic Biochemistry vols I and II. ed. G.L. Eichhorn, Elsevier.
4. Progress in Inorganic Chemistry, Vols 18 and 3S ed. J.J. Lippard, Wiley.
5. Bioorganic Chemistry: A Chemical Approach to Enzyme Action, Hermann Dugas and C. Penny, Springer-Verlag.
6. Understanding Enzymes, Trevor Palmer, Prentice Hall.
7. Enzyme Chemistry: Impact and Applications, Ed. Collin J Suckling, Chapman and Hail.
8. Enzyme Mechanisms Ed, M. 1. Page and A. Williams, Royal Society of Chemistry.
9. Fundamentals of Enzymology, N.C. Price and L. Slovens, Oxford University Press.
10. Immobilized Enzymes: An Introduction and Applications In Biotechnology, Michael 0. Trevan, John Wiley.
11. Enzymatic Reaction Mechanisms, C. Walsh, W. H. Freeman.
12. Enzyme Structure and Mechanism, A Fersht, W.H. Freeman.
13. Biochemistry: The Chemical Reactions of Living Cells, D. E. MeUler, Academic Press.

OR

PHOTO IN-ORGANIC CHEMISTRY

I Excited States of Metal Complexes **15 Hrs**

Excited states of metal complexes: comparison with organic compounds, electronically excited states of metal complexes, charge-transfer spectra, charge transfer excitations, methods for obtaining charge-transfer spectra.

II Ligand Field Photochemistry **15 Hrs**

Photosubstitution, photooxidation and photoreduction, lability and selectivity, zero vibrational levels of ground state and excited state, energy content of excited state, zerozero spectroscopic energy, development of the equations for redox potentials of the excited states.

III Redox Reactions by Excited Metal Complexes **25 Hrs**

Energy transfer under conditions of weak interaction and strong interaction-exciplex formation; conditions of the excited states to be useful as redox reactants, excited electron transfer, metal complexes as attractive candidates (2,2'-bipyridine and 1,10-phenonthroline complexes), illustration of reducing and oxidising character of Ruthenium^{2+}(bipyridal complex, comparision with $Fe(bipy)_3$; role of spin-orbit coupling-life time of these complexes. Application of redox processes of electronically excited

states for catalytic purposes, transformation of low energy reactants into high energy products, chemical energy into light

VI Metal Complex Sensitizers **15 Hrs**

Metal complex sensitizer, electron relay, metal colloid systems, semiconductor supported metal or oxide systems, water photolysis, nitrogen fixation and carbon dioxide reduction

Books Suggested

Concepts of Inorganic Photochemistry, A.W. Adamson and P.D. Fleischauer, Wiley.

2. Inorganic Photochemistry, J. Chem. Educ., vol. 60, no. 10, 1983.
3. Progress in Inorganic Chemistry, vol. 30, ed. S.J. Lippard, Wiley.
4. Coordination Chem. Revs., 1981, vol. 39, 121, 131; 1975, 15, 321; 1990, 97, 313.
5. Photochemistry of Coordination Compounds, V. Balzari and V. Carassiti, Academic Press.
6. Elements of Inorganic Photochemistry, G. J. Ferraudi, Wiley.

OR

ORGANIC

I Acids, Bases, Electrophiles, Nucleophiles and Catalysis **15 Hrs**

Acid-base dissociation. Electronic and structural effects, acidity and basicity. Acidity functions and their applications. Hard and soft acids and bases. Nucleophilicity scales. Nucleofugacity. The cx-effect. Ambivalent nucleophiles. Acid-base catalysis- specific and general catalysis. Bronsted catalysis. Nucleophilic and electrophilic catalysis. Catalysis by non- covalent binding-micellar catalysis.

II Steric and Conformational Properties **10 Hrs**

Various type of steric strain and their influence on reactivity. Steric acceleration. Molecular measurements of 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.

III Nucleophilic and Electrophilic Reactivity **10 Hrs**

Structural and electronic effects on S_N1 and S_N2 reactivity. Solvent effects. Kinetic isotope effects. Intramolecular assistance: Electron transfer nature of S_N2 reaction. Nucleophilicity and S_N2 reactivity based on curve- crossing model. Relationship between polar and electron transfer reactions. $_{SRO}$ mechanism. Elecrophilic reactivity, general mechanism. Kinetic of S_E2-Ar reaction. Structural effects on rates and selectivity. Curve-crossing approach to electrophilic reactivity.

IV Radical and Pericyclic Reactivity **10 Hrs**

Radical stability, polar influences, solvent and steric effects. A curve crossing approach to radical addition, factors effecting barrier heights in additions, regioselectivity in radical reactions, Reactivity, specificity and periselectivity in pericyclic reactions.

V Supramolecular Chemistry **25 Hrs**

Properties of covalent bonds - bond length, inter-bond angles, force constant, bond and molecular dipole moments. Molecular and bond polarizability, bond dissociation enthalpy,

entropy. Intermolecular forces, hydrophobic effects. Electrostatic, induction, dispersion and resonance energy. magnetic interactions, magnitude of interaction energy, forces between macroscopic bodies, medium effects. Hydrogen bond. Principles of molecular association and organization as exemplified in biological macromolecules like enzymes, nucleic acids, membranes and model systems like micelles and vesicles. Molecular receptors and design principles. Cryptands, cyclophanes, calixeranes, cyclodextrines. Supramolecular reactivity and catalysis. Molecular channels and transport processes. Molecular devices and nanotechnology.

OR

Pericyclic Reactions

Molecular orbital symmetry. Frontier orbitals of ethylene, 1, 3- butadiene. 1,3,5- hexatriene and allyl system classification of pericyclic reaction. Woodward Hoffman correlation diagrams. FMO and PMO approach. Electrolytic reactions- conrotatory and disrotatory motions. 4n, 4n+2 allyl systems. Cycloadditions- antarafacial and suprafacial additions. 4n and 4n+2 systems. Suprafacial and antarafacial shifts. Sigmatrophic arrangements. Claisen cope and azacope re-arrangements.

Books Suggested

1. Molecular Mechanics, U. Burkert and N. L. Allinger, ACS Monograph 177, 1982.
2. Organic Chemists' Book of Orbitals. L. Salem and W. L. Jorgensen,Academic Press.
3. Mechanism and Theory in Organic Chemistry, T. H. Lowry and K. C.Richardson, Harper and Row.
4. Introduction to Theoretical Organic Chemistry and Molecular.Modeling, W. B. Smith, VCH, Weinheim.
5. Physical Organic Chemistry, N. S. Isaacs, ELBS/Longman.
6. Supramolecular Chemistry, Concepts and Perspectives, J. M. Lehn, VCH.
7. The Physical Basis of Organic Chemistry, H. Maskill, Oxford University Press.

Chemistry
M.Sc. Semester-II
Core Course – 4 (CC-4)

Full Marks: 70+30
Time : 03 Hours

Total Lecturer : 70 Hours

Instruction to Question Setter:

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I. Quantum Chemistry — 30 Hrs

A Approximate Methods

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

B Angular Momentum

Ordinary angular momentum, generalized angular momentum, eigenfunctions for angular momentum, eigenvalues of angular momentum, operator using ladder operators, addition of angular momenta, spin, antisymmetry and Pauli exclusion principle.

C Electronic Structure of Atoms

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

D Molecular Orbital Theory

Huckel theory of conjugated systems, bond order and charge density calculations. Applications to ethylene, butadiene, cyclopropenyl radical, cyclobutadiene etc. Introduction to extended Hiackel theory.

II. Classical Thermodynamics **15 Hrs**

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. Determinations of these quantities. Concept of fugacity and determination of fugacity. Non-ideal systems: Excess functions for non-ideal solutions. Activity, activity coefficient, Debye-Huckel theory for activity coefficient of electrolytic solutions; determination of activity and activity coefficients; ionic strength. Gibb's Duhen equation, Nernst heat theorem and its applications, Determination of ablolute entropy Maxwell's thermodynamic relation.

III Chemical Dynamics **25 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. Dynamics of molecular motions, probing the transition state, dynamics of barrierless chemical reactions in solution, dynamics of unimolecular reactions (Lindemann - Hinshelwood and Rice-Ramsperger - Kassel-Marcus [RRKM] theories of unimolecular reactions).

Books Suggested

1. Physical Chemistry, P.W. Atkins, El

2. Introduction to Quantum Chemistry, A.K. Chandra, Tata McGraw Hill.
3. Quantum Chemistry, Ira N. Levine, Prentice Hall.
4. Coulson's Valence, R. McWeeny, ELBS.
5. Chemical Kinetics, K. J. Laidler, Mcgraw-Hill.
6. Kinetics and Mechanism of Chemical Transformations, J. Rajaraman and J. Kuriacose, McMillan.
7. Micelles, Theoretical and Applied Aspects, V. Moroi, Plenum
8. Modern Electrochemistry Vol. I and Vol. II, J.O.M. Bockris and A.K.N. Reddy, Plenum.
9. Introduction to Polymer Science, V.R. Gowarikar, N.V. Vishwanathan and J. Sridhar, Wiley Eastern.

Chemistry
M.Sc. Semester-II
Core Course – 5 (CC-5)

Full Marks: 70+30
Time : 03 Hours

Total Lecturer : 70 Hours

Instruction to Question Setter:

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End Semester Examination (ESE):
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(Attendance Upto75%, 1mark; 75<Attd.<80, 2 marks;80<Attd.<85, 3 marks;85<Attd.<90, 4 marks;90<Attd, 5 marks).

I Symmetry and Group Theory In Chemistry — 25 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, representations of groups by matrices (representation for the Cn, Cnv, Cnh. Dnh etc. groups to be worked out explicitly). Character of a representation. The great orthogonality theorem (without proof) and its importance. Character tables and their use; spectroscopy.

III Microwave Spectroscopy — 05 Hrs

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

IV Vibrational Spectroscopy — 20 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).

V Electronic Spectroscopy **10 Hrs**

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.

VI X-ray Diffraction **10 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 factor 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.

Books Suggested

1. Modern Speciroscopy, J.M. Hollas, John Wiley.
2. Applied Electron Spectroscopy lor Chemical Analysis Ed. H. Windawi and F.L. Ho. Wiley Interscience.
3. NMR, NOR, EPR and Massbauer Spectroscopy in Inorganic Chemistry, R.V. Parish, Ellis Harwood.
4. Physical' Methods in Chemistry, R.S. Drago, Saunders College.
5. Chemical Applications of Group Theory, F. A. Cotton.
6. Introduction to Molecular Spectroseopy, Q.M. Barrow, McCraw Hill.
7. Basic Principles of Spectroscopy. R. Chang, McOraw Hill.
8. Theory and Applications of UV Spectroscopy, H.H. Jatie and M. Orehin, IBH-Oxford.
9. Introduction to Photoelectron Spectroscopy, P. K. Ghosh, John Wiley.
10. Introduction to Magnetic Resonance, A. Carrington and A.D. Maclachalan, Harper & Row.

Chemistry
M.Sc. Semester-II
Core Corse (P) – 6 [CC(P)-6]

Full Marks: 100
Time : 06 Hrs

1. **Measurement of density of gases and vapours**
   (a) Victor Meyer's Method Determination of Molecular weight of Acetone, Chloroform, Benzene, (Mixture).
   (b) Duma's Method Determination of molecular weight of acetone, Carbon-Tetrachloride.
2. **Determination of Molecular weight of substances**
   (a) Beckmann's freezing point Method
   (b) Beckmann's Boiling point method.
3. **Viscosity of liquids and solution by ostwald tube**
   Determination of percentage composition of a mixture of two liquids.
4. **Surface Tension of liquids and solutions**
   (a) Study of the effect of conc. on surface tension of acetic acid and Sod. chloride solutions.
   (b) Determination of Parachor.
5. **Thermochemistry**
   (a) Determination of water equivalent of a calorimeter
   (b) Determination of the Heat of Neutralization of :
      (i) Strong acid and strong base (HCl and NaOH)
      (ii) Weak acid and strong base (NaOH and CH_3 COOH).
   (c) Determination of Heat of solution of Potassium Nitrate
   (d) Determination of basicity of succinic Acid by Thermochemical Method.
6. **Order of Reaction**
   (a) Determination of the rate constant of hydrolysis of an ester with an acid (Methyl acetate and HCl).
   (b) Determination of the rate constant of saponification of ethyl acetate by NaOH.
7. **Partition Co-efficient**
   (a) Determination of partition coefficient of:
      (i) Benzoic acid between water and Benzene
      (ii) Iodine between water and carbon tetrachloride
9. **Conductivity**
   (a) Determination of cell constant
   (b) Determination of equivalent conductivity of weak acid (acetic and succinic acid) at several concentrations and calculation of the dissociation constant of the acid
   (c) Determination of the basicity of an acid (citric acid and oxalic acid)
   (d) Titration of:
      (i) strong acid and strong base (HCl and NaOH)
      (ii) weak acid and strong base (CH_3COOH and NaOH)

Chemistry
M.Sc. Semester-III
Core Course – 7 (CC-7)

Full Marks: 70+30
Time : 03 Hours

Total Lecturer : 70 Hours

Instruction to Question Setter:

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(Attendance Upto75%, 1mark; 75<Attd.<80, 2 marks;80<Attd.<85, 3 marks;85<Attd.<90, 4 marks;90<Attd, 5 marks).

I Ultraviolet and Visible Spectroscopy — 10 Hrs

Various electronic transitions (185-800 nm), Beer—Lambert law, effect of solvent on electronic transitions, ultraviolet bands for carbonyl compounds, unsaturated carbonyl compounds, dienes, conjugated polyenes. Fieser-Woodward rules for conjugated dienes and carbonyl compounds, ultraviolet spectra of aromatic and heterocyclic compounds.

II Infrared Spectoscopy — 10 Hrs

Instrumentation and sample handling. Characteristic vibrational frequencies of alkanes, alkenes. alkynes, aromatic compounds, alcohols, ethers, phenols and amines. Detailed study of vibrational frequencies of carbony compounds (ketones, aldehydes, esters, amides, acids, anhydrides, lactones, lactams and conjugated carbonyi compounds). Effect of hydrogen bonding and solvent effect on vibrations frequencies, overtones, combination bands and Fermi resonance. FT IR. IR of gaseous, solids and polymeric materials.

III Nuclear Magnetic Resonance Spectroscopy — 14 Hrs

General introduction and definition, chemical shift, spin-spin interaction, shielding mechanism, chemical shift values and correlation for protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic) and other nuclei (alcohols, phenols, enols, carboxylic acids, amines, amides & mercapto), chemical exchange, effect of deuteration, solvent effects. Fourier transform technique.

Carbon-13 NMR Spectroscopy — **08 Hrs**

General considerations, chemical shift (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyi carbon), coupling constants. Two dimension NMR spectroscopy - COSY, NOESY. DEPT, INEPT, APT and INADEQUATE techniques.

IV Mass Spectrometry **10 Hrs**

Introduction, ion production - El, Cl, FD and FAB, factors affecting fragmentation, ion analysis, ion abundance. Mass spectral fragmentation of organic compounds, common functional groups, molecular ion peak, metastable peak, McLafferty rearrangement. Nitrogen rule. High resolution mass spectrometery. Examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

V Electron Spin Resonance Spectroscopy **09 Hrs**

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 PH_4, F_2^- and $[BH_3]^-$.

VI Mössbauer Spectroscopy **09 Hrs**

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

Books Suggested

1. Physical Methods lor Chemistry, R.S. Drago, Saunders Company.
2. Structural Melhods in Inorganic Chemistry, E.A.V. Ebsworth, D.W.H. Rankin and S. Cradock, ELBS
3. Infrared and Raman Spectra: Inorganic and Coordination Compounds, K. Nakamoto, Wiley.
4. Progress in Inorganic Chemistry vol., 8, ed., F.A. Cotton, vol., 15, ed. S.J. Lippard, Wiley.
5. Transition Metal Chemistry eA R.L. Carlin voi. S, Dekker
6. Inorganic Elecironie Speciroscopy,. A.P.B. Lever, Elsevier.
7. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R.V. Parish, Ellis Horwood.
8. Practical NMR Spoctroacopy, M.L Martin, J.J. Delpeuch and Q.J. fArtin, Heyden.
9. Spedrometric identitication of Organic Compounds, R. M. Silverstein, Q. C. gassier and T. C. Morrill, John Wiley
10. InirodlJCtion lo NMR Spectroscopy. R. J. Abraham, J. Fisher and P. Loftus, Wiley.
11. Application of Spectroscopy of Oiganic Compounds, J. R. Dyer, Prentice Hail.
12. Spectroscopic Methods in Organic Chemistry, D. H. Williams, 1. Fleming, Tala McGraw-Hill.

Chemistry
M.Sc. Semester-III
Core Course – 8 (CC-8)

Full Marks: 70+30
Time : 03 Hours

Total Lecturer : 70 Hours

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(Attendance Upto75%, 1mark; 75<Attd.<80, 2 marks;80<Attd.<85, 3 marks;85<Attd.<90, 4 marks;90<Attd, 5 marks).

I Environment — 10 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.

II Hydrosphere — 20 Hrs

Chemical composition of water bodies-lakes, streams, rivers and wet lands etc. 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 BOO, DO, COD, F, Oils, metals (As, Cd, Cr, Hg, Pb, Se etc.), residual chloride and chloine demand. Purification and treatment of water.

III Soils **05 Hrs**

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

IV Atmosphere **15 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, 0 and their effect, pollution by chemicals, petroleum, minerals, chlorofluorohydrocarbons. Green house effect, acid rain, air pollution controls and their chemistry. Analytical methods for measuring air pollutants. Continuous monitoring instruments.

V Industrial Pollution **10 Hrs**

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

VI Environmental Toxicology **10 Hrs**

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

Books Suggested

Environmental Chemistry, S. E. Manahan, Lewis Publishers.

Environmental Chemistry, Sharma & Kaur, Krishna Pubilshers.

Environmenlal Chemistly, A. K. De, Wiley Easlem.

Environmental Pollution Analysis, S.M. Khopkar, Wiley Eastern

Standard Method of Chemical Analysis, FJ. Weleher Vol. III. Van Nostrand Reinhold Co.

Environmental Toxicology, Ed. J. Rose, Gordon and Breach Science Publication.

Elemental Analysis of Airborne Particles, Ed. S. Landsberger and M. Crealchman, Gordon and Breach Science Publication.

Environmentai Chemistry, C. Baird, W. H. Freeman.

Chemistry
M.Sc. Semester-III
In-Organic
Elective (GE/DC) (EC-2)

Full Marks: 70+30
Time : 03 Hours

Total Lecturer : 70 Hours

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I **Alkyls and Aryls of Transition Metals** **05 Hrs**
Types, routes of synthesis, stability and decomposition pathways, organocopper in organic synthesis

II **Compounds of Transition Metal-Carbon Multiple Bonds** **15 Hrs**
Alkylidenes, alkylidynes, low valent carbenes and carfaynes- synthesis, nature of bond, structural characteristics, nucleophilic and electrophilic reactions on the ligands, role in organic synthesis

III **Transition Metal p-Complexes** **18 Hrs**
Transition meta! n-complexes with unsaturated organic molecules, alkenes, alkynes, atlyl, diene, dienyl, arene and trienyt complexes, preparations, properties, nature of bonding and structural features. Important reactions relating to nucleophilic and electrophilic attack on ligands and to organic synthesis

IV **Transition Metal Compounds with Bonds to Hydrogen** **07 Hrs**
Transition Metal Compounds with Bonds to Hydrogen.

I **Metals in Medicine** **05 Hrs**
Metal deficiency and disease, toxic effects of metals, metals used for diagnosis and chemotherapy with particular reference to anticancer drugs

III Homogeneous Catalysis **14 Hrs**

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

IV Pluxional Organometalilc Compounds **06 Hrs**

Fluxionality and dynamic equilibria in compounds such as h^2- olefin, h^3 allyl and dienyl complexes

Books Suggested

1 Principles and Application of Organotransition Metal Chemistry, J.P. Collman, L.S. Hegsdus, J.R. Norton and R.G. Pinke, University Science Books.
2 The Organometaltic Chemistry o1 the Transition Metals, R.H. Crabtree, John Wiley
3 Metallo-organic Chemistry, A.J. Pearson, Wiley.
4 Organometallic Chemistry, R.C. Mehrotra and A. Singh, New Age International.

Chemistry
M.Sc. Semester-III
Organic
Elective (GE/DC) (EC-2)

Full Marks: 70+30
Time : 03 Hours

Total Lecturer : 70 Hours

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I Terpenoids and Carotenoids **15 Hrs**

Classification, nomenclature, occurrence, isolation, general methods of structure determination, isoprene rule. Structure elucidation, stereochemistry, biosynthesis and synthesis of

the following representative molecules: Citral, a-Terpeneol, Zingiberene, Santonin, Bisabolene acid and (3-Carotene.

II Alkaloids **14 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, Narcotine, Reserpine

III Six-Membered Heterocycles with one Heteroatom **06 Hrs**

Synthesis and reactions ofpyrytium salts and pyrones and their comparison with pyridinium & thiopyrylium salts and pyridones. Synthesis and reactions of quinolizinium and benzopyrylium salts, coumarins and chromones

IV Heterocyclic Systems Containing S & As **12 Hrs**

Heterocyclic rings containing phosphorus: introduction, nomenclature, Synthesis and characteristics of 5- and 6-membered ring systems-phosphorinanes, phosphorines, phospholanes and phospholes.Heterocydic rings containing As introduction, synthesis and characteristics of 5- and 6 membered ring systems.

II Principles of Reactivity **07 Hrs**

Mechanistic significance of entropy, enthalpy and Gibb's 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.

III Kinetic Isotope Effect **06 Hrs**

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

IV Structural Effects on Reactivity **10 Hrs**

Linear free energy relationships (LFER). The Hammett equation, substituent constants, theories of substituent effects. Interpretation of (5-values. Reaction constant p. Deviations from Hammett equation. Dual-parameter correlations, inductive substituent constant. The

Taft model, $6,$- and cT_R-scales.

Books Suggested

1. Molecular Mechanics, U. Burkert and N. L. Allinger, ACS Monograph 177, 1982.
2. Organic Chemists' Book of Orbitals. L. Salem and W. L. Jorgensen,Academic Press.
3. Mechanism and Theory in Organic Chemistry, T. H. Lowry and K. C.Richardson, Harper and Row.
4. Introduction to Theoretical Organic Chemistry and Molecular.Modeling, W. B. Smith, VCH, Weinheim.

5. Physical Organic Chemistry, N. S. Isaacs, ELBS/Longman.
6. Supramolecular Chemistry, Concepts and Perspectives, J. M. Lehn, VCH.
7. The Physical Basis of Organic Chemistry, H. Maskill, Oxford University Press.

Chemistry
M.Sc. Semester-III
Physical
Elective (GE/DC) (EC-2)

Full Marks: 70+30
Time : 03 Hours

Total Lecturer : 70 Hours

Instruction to Question Setter:

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I Diffraction of X-rays by crystals — 08 Hrs

Debye Scherrer mechod, indexing powder pattern for cubic and tetragonal crystals, rotating crystal method, Fourier transform and reciprocal lattices, Bragg equation in reciprocal lattice, neutron diffraction.

II Metallic bonds — 15 Hrs

Free electron theory, band theory, Fermi level, Brillouin zone, wave function for electrons in solids, metallic conductors, insulator, semi conductors (intrinsic & extrinsic), properties of junctions.

III Polymer — 09 Hrs

Polymer solution, thermodynamics of polymer solutions, molar mass and molar mass distribution, methods of measuring molar masses , micelle formation and hydrophobic interaction.

IV Electrically conducting polymers — 08 Hrs

Electrically conducting polymers electrochemical polymerization, band structure of polymers, mechanism of conduction in polymers, doping of polymers, application of conduction polymers.

V Potential Energy Surfaces **15 Hrs**

Mechanism of activation, potential energy surface for three atom reaction, Potential energy curve for successive reations, Propertions of potential energy surfaces, Inter conversion of translational and vibrational energies, Combination of atoms, Orthopara conversion, Activated state of three atom and four atom reactions, Potential energy rpfile, reaction co-ordinate, Transmission co-efficient, non-adiabatic reaction.

VI Study of Fast Reactions **15 Hrs**

Photo physical Chemistry-Flash Photolysis, Relaxation technique, Nuclear Magnetic Resonance Method, Molecular Beam and Shock-tube Kinetics, Flow method. Reactions of Protons, Electrons metal ions.

Chemistry
M.Sc. Semester-III
In-Organic
EC(P)-3

Full Marks: 100
Time : 06 Hrs

Credit : 5

1. Qualitative separation and determination of the following pairs of metal ion using gravimetric and volumetric methods
   a) $Ag^{+}(g)$ and $Cu^{2+}(v)$
   b) $Cu^{2+}(g)$ and $Zn^{2+}(v)$
   c) $Fe^{3+}(g)$ and $Ca^{2+}(v)$
   d) $Mg^{2+}(g)$ and $Ca^{2+}(v)$
2. Semi micro qualitative analysis of a mixture containing five cations of rare element and insolables.
   a) Rare element Tl, W Sc Mo, Ti, Zr Ce, Tb V, V, Lx
   b) Insoluble $PbSO_4$, $SrSO_4$, Al_2O_3 Cr_2O_3, Fe_2O_3, SnO_2, ThO_2, WO_3

Chemistry
M.Sc. Semester-III
Organic
EC(P)-3

Full Marks: 100
Time : 06 Hrs

Credit : 5

Group A

Characterization of organic compounds, The students expected to carry out analysis of the components of binary org. mixture (liquid-liquid, liquid-solid & solid-solid) the students should also chek the purity of the separated components on TLC plates.

Group-B

1. To determine the percentage or number of phenolic groups in the given sample by the acetylation method.
2. To determine the percentage or number of methoxyl groups in the gtiven sample by the Zeisel's method.
3. To determine the iodine number of the given fat or oil sample.

Chemistry
M.Sc. Semester-III
Physical
EC(P)-3

Full Marks: 100
Time : 06 Hrs

Credit : 5

I Conductometry

1. To determine the solubility and solubility product of a sparingly soluble salt
2. To verify Onsager equation for a uni-univalent electrolyte in aqueous solution
3. To titrate a mixture of HCl, CH_3COOH and $CuSO_4$ with NaOH
4. To determine the rate constant of saponification of an ester by NaOH.

II. Potentiometry

1. To determine the solubility and solubility product of AgCl in water
2. To determine the E^0 of Zn/Zn^{++}, Cu/Cu^{++} ELECTRODES.
3. To determine the basicity of a polybasic acid and its dissociation constant.
4. To investigate the complex formed between $CuSO_4$ and NH_3.

III. Polarimetry

1. To analyse a mixture of glucose and sucrose
2. To study the inversion of cane sugar in acid medium.

IV. Refractometry

1. To verify mixture law of refraction
2. To determine the composition of an unknown solution.

V. Cryoscopy

1. To determine the activity of a non-electrolyte by freezing point method
2. To determine the mean activity co-efficient of KCl by freezing point method.

Chemistry
M.Sc. Semester-IV
CC-9

Full Marks: 70+30
Time : 03 Hours

Total Lecturer : 70 Hours

Instruction to Question Setter:

Mid Semester Examination (MSE):
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End Semester Examination (ESE):
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Note: *There may be subdivisions in each question asked in Theory Examinations*
*The Mid Semester Examination shall have three components. (a) Two Semester Internal Assessment Test (SIA) of 20 Marks each, (b) Class Attendance Score (CAS) of 5 marks and (c) Class Performance Score (CPS) of 5 marks. "**Better of Two**" shall be applicable for computation of marks for SIA.*

(Attendance Upto75%, 1mark; 75<Attd.<80, 2 marks;80<Attd.<85, 3 marks;85<Attd.<90, 4 marks;90<Attd, 5 marks).

I **Introduction** **15 Hrs**

Role of analytical chemistry. Classification of analytical methods-classical and instrumental. Types of instrumental analysis. Selecting an analytical method. Neatness and cleanliness. Laboratory operations and practices. Analytical balance. Techniques of weighing, errors. Volumetric glassware-cleaning and calibration of glassware. Sample preparations - dissolution and decompositions. Gravimetric techniques. Selecting and handling of reagents. Laboratory notebooks. Safety in the analytical laboratory.

II **Errors and Evaluation** **15 Hrs**

Definition of terms in mean and median. Precision-standard deviation, relative standard deviation. Accuracy-absolute error, relative error. Types of error in experimental data-determinate (systematic), indeterminate (or random) and gross. Sources of errors and the effects upon the analytical results. Methods for reporting analytical data. Statistical evaluation of data-indeterminate errors. The uses of statistics.

III **Food Analysis** **12 Hrs**

Moisture, ash, crude protein, fat, crude fibre, carbohydrates, calcium, potassium, sodium and phosphate. Food adulteration-common adulterants in food, contamination of food stuffs. Microscopic examination of foods for adulterants. Pesticide analysis in food products. Extraction and purification of sample. HPLC. Gas

chromatography for organophosphates. Thin-layer chromatography for identification of chlorinated pesticides in food products.

IV Analysis of Water Pollution **16 Hrs**

Origin of waste water, types, water pollutants and their effects. Sources of water pollutiondomestic, industrial, agricultural soil and radioactive wastes as sources of pollution. Objectives *of* analysis-parameter for analysis-colour, turbidity, total solids, conductivity, acidity, alkalinity, hardness, chloride, sulphate, fluoride, silica, phosphates and different forms of nitrogen. Heavy metal pollution-public health significance of cadmium, chromium, copper, lead, zinc, manganese, mercury and arsenic. General survey of instrumental technique for the analysis of heavy metals in aqueous systems. Measurements of DO, BOD and COD. Pesticides as water pollutants and analysis. Water pollution laws and standards.

V Analysis of Soil, Fuel, Body Fluids and Drugs **12 Hrs**

(a) Analysis of soil: moisture, pH, total nitrogen, phosphorus, silica, lime, magnesia, manganese, sulphur and alkali salts.

(b) Fuel analysis: solid, liquid and gas. Ultimate and proximate analysis-heating valuesgrading of coal. Liquid fuels-flash point, aniline point, octane number and carbon residue. Gaseous fuels-producer gas and water gas-calorific value.

(c) Clinical chemistry: Composition of blood-collection and preservation of samples. Clinical analysis. Serum electrolytes, blood glucose, blood urea nitrogen, uric acid, albumin, globulins, barbiturates, acid and alkaline phosphatases. Immunoassay: principles of radio immunoassay (RIA) and applications. The blood gas analysistrace elements in the body.

(d) Drug analysis: Narcotics and dangerous drugs. Classification of drugs. Screening by gas and thin-layer chromatography and spectrophotometric measurements.

Books Suggested

1. Analytical Chemistry, G.D. Christian, J. Wiley.
2. Fundamentals of Analytical Chemistry, D.A. Skoog, D.M. West and F.J. Holler, W. B. Saunders.
3. Analytical Chemistry-Principles, J.H. Kennedy, W. B. Saunders.
4. Analytical Chemistry-Principles and Techniques, L.G. Hargis, Prentice Hall.
5. Principles of Instrumental Analysis, D.A. Skoog and J.L. Loary, W. B. Saunders.
6. Principles of Instrumental Analysis, D.A. Skoog, W. B. Saunders.
7. Quantitative Analysis, R.A. Day, Jr. and A.L. Underwood, Prentice Hall.
8. Environmental Solution Analysis, S.M. Khopkar, Wiley Eastern
9. Basic Concepts of Analytical Chemistry, S.M. Khopkar, Wiley Eastern
10. Handbook of Instrumental Techniques for Analytical Chemistry, F. Settle, Prentice Hall.
11. Analytical Chemistry, G.D. Christian, J. Wiley.

Chemistry
M.Sc. Semester-IV
In-Organic
Elective (GE/DC) [EC-4]

Full Marks: 70+30
Time : 03 Hours

Total Lecturer : 70 Hours

Instruction to Question Setter:

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(Attendance Upto75%, 1mark; 75<Attd.<80, 2 marks;80<Attd.<85, 3 marks;85<Attd.<90, 4 marks;90<Attd, 5 marks).

I Metal Storage Transport and Biomineralization **07 Hrs**

Ferritin, transferrin, and siderophores

II Calcium in Biology **10 Hrs**

Calcium in living cells, transport and regulation, molecular aspects of intramolecular processes, extracellular binding proteins

III Metalloenzymes **20 Hrs**

Zinc enzymes - carboxypeptidase and carbonic anhydrase. Iron enzymes - catalase, peroxidase and cytochrome P-450. Copper enzymes - superoxide dismutase. Molybdenum oxatransferase enzymes - xanthine oxidase. Coenzyme vitamin BII

IV Metal-Nucleic Acid Interactions **08Hrs**

Metal ions and metal complex interactions. Metal complexes - nucieic acids

II Supramolecular Chemistry **25 Hrs**

Concepts and language.

(A) Molecular recognition : 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 devices. Supramolecular photochemistry, supramolecular electronic, ionic and switching devices.

Some example of self-assembly in supramolecular chemistry

Books Suggested

1 Principles of Bioinorganic Chemistry, S.J. Lippard and J.M. Berg, University Science Books.

2 Bioinorganic Chemistry, 1. Bertini, H.B. Gray, S.J. Lippard and J.S. Valentine, University Science Books.

3 Inorganic Biochemistry vols I and II. ed. 0.L Eichhom, Elsevier.

4 Progress in inorganic Chemistry, Vols 18 and 38 ed. J.J. Lippard, Wiley.

5 Supramolecular Chemistry, J.M. Lehn, VCH.

Chemistry
M.Sc. Semester-IV
Organic
Elective (GE/DC) [EC-4]

Full Marks: 70+30
Time : 03 Hours

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I Steroids **20 Hrs**

Occurrence, nomenclature, basic skeleton, Diel's hydrocarbon and stereochemistry. Isolation, structure determination and synthesis of Cholesterol, Bile acids, Androsterone, Testosterone, Estrone, Progestrone, Biosynthesis of steroids.

II Six-Membered Heterocycles with Two or More Heteroatoms **05Hrs**

Synthesis and reactions of diazines, triazines, tetrazines and thiazines

III Seven- and Large-Membered Heterocycles **05 Hrs**

Synthesis and reactions of azepines, diazepines.

IV Structure Determination and Synthesis of Vit. A, B1, B_2, B_6, Vit. C and Vit. D. 20 Hrs

V Concepts in Molecular Orbital (MO) and Valence Bond (VB) Theory 20 Hrs

Introduction to Huckel molecular orbital (MO) method as a means to explain modern theoretical methods. Advanced techniques in PMO and FMO theory. Molecular mechanics,

semi empirical methods and *ab inito* and density functional methods. Scope and limitations of several computational programmes.

Quantitative MO theory - Huckel molecular orbital (HMO) method as applied to ethene, allyl and butadiene. Qualitative MO theory - ionisation potential. Electron affinities. MO energy levels. Orbital symmetry. Orbital interaction diagrams. MO of simple organic systems such as ethene, allyl, butadiene, methane and methyl group. Conjugation and hyperconjugation. Aromaticity.

Valence bond (VB) configuration mixing diagrams. Relationship between VB configuration mixing and resonance theory. Reaction profiles. Potential energy diagrams. Curvecrossing model-nature of activation barrier in chemical reactions

Books Suggested

1. Heterocyclic Chemistry Vol. 1-3, R. R. Supta, M. Kumar and V Gupta, Springer Verlag.
2. The Chemistry ofHeterocycles, T. Eicher and S. Hauptmann, Thieme.
3. Heterocyclic Chemistry, J. A. Joule, K. Mills and G.F. Smith, Chapman and Hall.
4. Heterocyclic Chemistry.T.L Gilchrisl.Longman Scietific Teehinai
5. Contemporary Heterocyclic Chemisiry, Q. R. Newkome and W. W. Paudler, Wiley-inter Science.
6. An introduction to the Heterocyclic Compounds. Linds, R. M. Acheson, JohnWiley.
7. Comprehensive Heterocyclic Chemistry, A. R. Kalriliky and C. W. Rees, eds. Pergamon Press.
8. Natural Produds; Chemistry and Biological Significance, J. Mann, R. S. Davidson, J.B.Hobbs, D.V, Banthirope and J. B. Harbome, Longman,Essex.
9. Organic Chemistry, Vol 2, I. L. Finar, ELB S.
10. Stereoselective Synthesis; A Practical Approach, M.Nogradi.VCH.
11. Rodd's Chemistry of Carbon Compounds. Ed. S. Coffey, Elsevier.
12. Chemistry, Biological and Pharmacological Properties of Medicinal lants from the Americas, Ed. Kurt Hosiettmann, M. P. Gupla and A. Marston, Harwood Academic Publishers.
13. Introduction lo Flavonoids. B.A. Bohm, Harwood Academic Publishers.
14. New Trends in Natural Product Chemistry, Atta-ur-Rahman and M I Choudhary, Harwood Academic Publishers.

Chemistry
M.Sc. Semester-IV
Physical
Elective (GE/DC) [EC-4]

Full Marks: 70+30
Time : 03 Hours

Total Lecturer : 70 Hours

Instruction to Question Setter:

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I **Super conductivity** **11 Hrs**

Super conductivity meissner effect, microscopic theory of superconductivity, conventional organic and high temp, superconductors, fullerenes, applications of superconductors.

Transformation in crystals - thermodynamics of transformation, order-disorder transitions, martensitic transition, polymorphic transformation

II **Specific heat of solids** **11 Hrs**

Specific heat of solids classical theory, quantum theory of specific heats-Einstein and Debye theories, characteristic temp and its calculation, T-law. Solid state reactions, laws governing nucleation, homogeneous and heterogenous nucleation, thermodynamic barrier.

III **Polymer liquid crystal** **11 Hrs**

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

IV Surface chemistry 12 Hrs

Surface chemistry surface films, BET isotherm for, multilayers & its derivation, kinetics of surface processes, unimolecular and bimolecular surface reactions, electrocapillarity, electrokinetic effects, statistical mechanics of adsorption.

VI Kinetics of Condensed Phase Reactions 25 Hrs

Rate determining steps in diffusion controlled 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 ontribution to free energy in single and double spherical models of activated comlex, entropy of activation for ion-ion reactions; Kinetics of dipole-dipole reaction, ion-dipole reaction, dependence of rate constant on ionic strength and dielectric constant of medium, Bronsted-Bjerrum equation.

Books suggested

1. Crystallography - Philips
2. Solid State chemistry-Garner (Butterworth; London)
3. Solid State Chemistry -D.K.Chakraborty (New Age int Publication)
4. Solid State Chemistry- N. BHannay (Prentice Hall, New Jersay)
5 Physical Chemistry- Waller J. Moore
6 Physical Chemistry - P.W. Atkins
7. Principles of polymer chemistry Cornell , P. J. Flory (Univ. Press)
8. Handbook of Conducting Polymers Vol I & II" T A. Skolhia.

Chemistry
M.Sc. Semester-IV
In-Organic
EC(P)-5

Full Marks: 100
Time : 06 Hrs

Credit : 5

I Quantitative Analysis

(i) Analysis of alloys (brass, type metal, solder, gun metal) cement, steel using conventional chemical analysis/and physical techniques (if possible). (Preferably one alloy and cement analysis may be carried out).

(ii) Analysis of two cation-system using complexones.

(iii) Colorimetric estimation of cation/anions.

II Separation Techniques

(i) Ion exchange: Separation of inorganic cations/anions (2 or 3 components).

(ii) Chromatographic Separation.

(a) Cd-Zn (b) Zn-Mg

III Preparation of six to eight simple inorganic complexes, their purification, Molecular Weight determination and elucidation of the structures by available physical methods

(a) Preparation of Cobalt (III) complexes

(i) $[Co(NH_3)_5 Cl] Cl_2$

(ii) $[Co(NH_3)_5 NO_2] Cl_2$

(iii) $[Co(NH_3)_5 ONC] Cl_2$

(b) Preparation and characterisation of Cr(III) complexes

(i) $[Cr(H_2O)_6] NO_3 H_2O$

(ii) $[Cr(H_2O)_4 Cl_2] Cl H_2O$

(iii) $Cr(acac)_3$

(c) (i) Purification of inorganic complexes using techniques such as crystallisation, volatilisation etc.

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

(d) Preparation and study of cis and trans isomers of bis (glycinato) copper(II)

(i) Cis-glycinato Cu(II) monohydrate

(ii) trans-glycinato Cu(II) monohydrate (IR sepectroscopy)

(e) Preparation of mercury tetrathiocyanato cobaltate : $Hg[Co(CNS)_4]$

IV Flame Photometric Determinations

(a) Sodium and Potassium when present together

(b) Li/Ca/Ba/Sr Naphelometric determinations

(a) Sulphate (b) Phosphate (c) Silver

V Determination of

(a) Manganese/Chromium/Vanadium in steel sample by spectrophotometric method

(b) Ni/Mo/W/V/U by extractive spectrophotometric method.$_3$

Chemistry
M.Sc. Semester-IV
Organic
EC(P)-5

Full Marks: 100
Time : 06 Hrs

Credit : 5

I Organic Systhesis and Extraction of Organic Compounds from Natural Sources

The students are expected to carry out 6 to 8 organic preparations (usually involving not more than two steps). Some of the illustrative experiments are listed below:

1. Extraction of Caffeine from Tea Leaves (Ref. Experimental Organic Chemistry H Dupon Durst. George W.Gokel, p.464 McGraw Hall Book Co., New York).

   Student should be asked to purify the crude sample, check the purity on a TLC single spot and/or get the pmr scanned and interpret. (Three methyl singles and 1 methine singlet).
2. Isolation of casein from milk (Try some typical colour reactions of proteins).
3. Isolation of lactose from milk (check purity of sugar by TLC and PC and calculate Rf value).
4. Isolation of nicotine dipicrate from tobacco.
5. Synthesis of 3-nitrobenzoic acid from benzoic acid.(Ref.: ibid,p. 246-247 and 443-448)

   Aim To demonstrate the process of metanitration, esterification and saponification of an ester.

   Make a comparative study of IR and PMR spectra of benzoic acid, methyl benzoate, methyl 3-nitrobenzoate, if possible.
6. Preparation of Indigo from anthranilic acid
7. Cannizzaro reaction of 4-chlorobenzaldehyde (Ref: ibid, p.397-400).

   Aim To demonstrate technique of isolation of two products from the reaction mixture and the procedure of intermolecular hydride transfer.

   Make a comparative study of IR PMR spectra of 4-Chlorobenzyl alcohol if possible.
8. Synthesis of benzanilide from benzene (Ref: ibid, p.775, 812)

   Aim To carry out Friedel Crafts acylation (anhydrous conditions) and Beckman rearrangement. Make a comparative study of the IR and PMR spectra of benzene,

benzophenone, benzophenone oxime and benzanilide (N-H stretching vibrations typical of a secondary amide) if possible.

II Characterization of organic compounds. The students is expected to carry out anlysis of the components of binary organic mixture (liquid-liquid, liquid-solid and solid-solid). Using chemical analysis and/or IR, and PMR data. The student should also check the purity of the separated components on TLC plates.

III **Quantative Analysis**

Some illustrative exercises are given below:

1. Estimation of phenol / aniline using bromate bromide solution/or acetylation method
2. Estimation of carbonyl group by using 2,4-dinitrophenyl hydrazine
3. To estimate nitrogen in the given sample by Kjeldahl method
4. To estimate sulphur in the given sample by the Na_2CO_3-KNO_3 fusion method.
5. To estimate sulphur in the given sample by Messenger's method.
6. To estimate a halogen in the given sample by the alkaline reduction method (modified Stepanow method).
7. To determine the percentage or number of hydroxyl groups in the given sample by the acetylation method.

Chemistry
M.Sc. Semester-IV
In-Organic
EC(P)-5

Full Marks: 100
Time : 06 Hrs

Credit : 5

I Chemical Kinetics

1. To study the kinetics of alkaline hydrolysis of an ester in aquo-organic solvent system with respect to effect of solvent composition and dielectric constant on rate constant.
2. To determine the rate constant of the reaction between $K_2S_2O_8$ and KI at two different temp. and hence to determine the energy of activation of the reaction.

II. Thermochemistry

1. Determination of basicity of a polybasic acid.
2. Determination of heat of displacement of Cu by Zn from Cu^{2+} salt solution.
3. Determination of heat of hydration of Na_2SO_4 to Na_2SO_4, 10 H_2O.

III. Distribution law

1. Determination of Composition of Cupric-ammine sulphate formed between $CuSO_4$ and NH_3
2. Determination of equilibrium constant for the reaction $KI+I_2=KI_3$

IV. Thermodynamics and Surface Chemistry

1. To study the adsorption of acetic acid on charcoal
2. To determine the partial molar volume of solutions of simple salts and to study its variation with concentration

V. Viscosity and Surface Tension

1. To determine the radius of a molecule from viscosity measurement.
2. To determine the parachor of - CH_2, C and H

Chemistry

M.Sc. Semester-IV

Project

Full Marks: 100

Credit: 5

Group A: 30 Marks

Group B: 70 marks

Group A-

I. IPR (Intellectual Property Right)
   i. Introduction & need for IPR, kinds of IPR
   ii. Patents- Registration procedures, rights & duties of Patents, introduction to Indian Patent Law
   iii. India's New National IP Policy 2016- Govt. of India step towards promoting IPR

II. Research Methodology
   i. Introduction to Research
   ii. Statement of the Problem & Hypothesis
   iii. Experimental & non-experimental research design

Group B- Project Work