

DR. SHYAMA PRASAD MUKHERJEE UNIVERSITY, RANCHI

UNIVERSITY DEPARTMENT OF CHEMISTRY

M.Sc. Programme in Chemistry

(Based on CBCS Pattern)

Guideline and syllabus for 2 years M.Sc. Programme in Chemistry

2018-20 onwards

APPROVED BY

THE BOARD OF STUDIES,

UNIVERSITY DEPARTMENT OF CHEMISTRY

DR. SHYAMA PRASAD MUKHERJEE UNIVERSITY, RANCHI

UNIVERSITY DEPARTMENT OF CHEMISTRY

BOARD OF STUDIES

FOREWORD

A Meeting of the BOARD OF STUDIES was held in the UNIVERSITY DEPARTMENT OF CHEMISTRY, DSPM UNIVERSITY, RANCHI on 24.04.2018. All Members participated in the syllabus approval meeting. The Draft Syllabus for M.Sc. Programme in Chemistry was approved. It will be placed before the ACADEMIC COUNCIL of DSPM UNIVERSITY for final approval.

- 1. Prof. R. R. Jha** External Subject Expert
Former Head
University Department of Chemistry,
RU, Ranchi
- 2. Prof. Sanjoy Misra** External Subject Expert
Former Head
University Department of Chemistry,
RU, Ranchi
- 3. Dr. N. K. Roy** Faculty Member
Assistant Professor
University Department of Chemistry,
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- 4. Dr. A. K. Acharya** Faculty Member
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University Department of Chemistry,
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- 5. Dr. Rajeev Ranjan** Faculty Member
Assistant Professor
University Department of Chemistry,
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- 6. Dr. Poonam Bhardwaj** Faculty Member
Assistant Professor
University Department of Chemistry,
DSPMU, Ranchi
- 7. Dr. Khurshid Akhtar** Chairperson & HOD
Assistant Professor
University Department of Chemistry,
DSPMU, Ranchi

FOREWORD

In the UNIVERSITY DEPARTMENT OF CHEMISTRY, DSPM UNIVERSITY, the faculty members participated in the syllabus preparation meetings held on 15.02.2018, 17.02.2018, 19.02.2018, 21.02.2018, 21.02.2018 and 24.02.2018. Keeping in view the aims of the UGC Model Curriculum in developing interdisciplinary skills in students, linking chemistry studies with professional development of students and also catering to present industrial needs, the teachers of different branches of chemistry, namely Inorganic, Organic and Physical chemistry had joint brainstorming sessions and arrived at a Draft Syllabus in Chemistry for Four semesters M.Sc. course. The Draft Syllabus was then approved by the Department Council in a meeting held on 26.02.2018 and placed before the Board of Studies of UNIVERSITY DEPARTMENT OF CHEMISTRY, DSPM University, Ranchi for approval.

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|--|------------------------------|
| 1. Dr. N. K. Roy
Assistant Professor
University Department of Chemistry,
DSPMU, Ranchi | Faculty Member |
| 3. Dr. Rajeev Ranjan
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| 5. Dr. Khurshid Akhtar
Assistant Professor
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GENERAL GUIDELINES

1. M.Sc. Course in Chemistry shall be of two years duration.
2. There shall be semester wise examination.
3. There shall be four semester (04) in two years, Semester-I and Semester-II in first year (1st year) and Semester-III and Semester-IV in the second year (2nd year).
4. There shall be three theory papers of 100 marks each of THREE HOURS duration and one practical exam of 100 marks of SIX HOUR duration in each Semester-I, II & III. In Semester-IV, there will be one PROJECT WORK of 100 MARKS. There shall be a Mid Term Examination also in each Semester of 30 marks in each theory papers.
5. There shall be 11 theory papers, 4 practical papers and 1 Project Work altogether.
6. There shall be THREE GROUPS of optional elective paper, out of which student has to elect ONE GROUP.

GROUP OF ELECTIVE PAPERS:

Group-A : INORGANIC CHEMISTRY
Group-B : ORGANIC CHEMISTRY
Group-C : PHYSICAL CHEMISTRY

7. Each theory paper in each END SEMESTER EXAMINATION shall carry SEVENTY (70) as FULL MARKS.
8. There shall be MID SEMESTER EXAMINATION/ INTERNAL EVALUATION in the middle of each Semester carrying THIRTY (30) as FULL MARKS.
9. There shall be total EIGHT (08) questions in each End-Semester Examinations. Examinees are required to answer any FIVE (05) questions out of EIGHT (08).
10. The duration of End-Semester Examination shall be of THREE (03) HOURS in each theory paper of each Semester.

Course Structure for M.Sc. Programme in Chemistry

SEM	COURSE OPTED	Paper	Distribution of Marks			
			END SEM	MID SEM	PRACTICAL / PROJECT	TOTAL
I	FC (Compulsory) – (FC-I)	1	70	30	-	100
	Core Course – 1 (CC-1)	2	70	30	-	100
	Core Course – 2 (CC-2)	3	70	30	-	100
	Core Course (P) – 3 [CC (P)-3]	4	-	-	100	100
II	Elective Course (SE) (EC-1)	5	70	30	-	100
	Core Course – 4	6	70	30	-	100
	Core Course – 5	7	70	30	-	100
	Core Course (P) – 6 [CC (P)-6]	8	-	-	100	100
III	Core Course – 7	9	70	30	-	100
	Core Course – 8	10	70	30	-	100
	Elective (GE/DC) (EC-2)	11	70	30	-	100
	Elective Course (P) – 3 [EC (P)-3]	12	-	-	100	100
IV	Core Course – 9	13	70	30	-	100
	Elective (GE/DC) (EC-4)	14	70	30	-	100
	Elective Course (P) – 5 [EC (P)-5]	15	-	-	100	100
	Project	16	-	-	100	100

Semester-wise Distribution of Course

SEM	COURSE	CREDIT	Hrs./Week
I	FC (Compulsory) – (FC-I)	5	5 (L) + 1 (T)
	Core Course – 1 (CC-1)	5	5 (L) + 1 (T)
	Core Course – 2 (CC-2)	5	5 (L) + 1 (T)
	Core Course (P) – 3 [CC (P)-3]	5	10
II	Elective Course (SE) (EC-1)	5	5 (L) + 1 (T)
	Core Course – 4	5	5 (L) + 1 (T)
	Core Course – 5	5	5 (L) + 1 (T)
	Core Course (P) – 6 [CC (P)-6]	5	10
III	Core Course – 7	5	5 (L) + 1 (T)
	Core Course – 8	5	5 (L) + 1 (T)
	Elective (GE/DC) (EC-2)	5	5 (L) + 1 (T)
	Elective Course (P) – 3 [EC (P)-3]	5	10
IV	Core Course – 9	5	5 (L) + 1 (T)
	Elective (GE/DC) (EC-4)	5	5 (L) + 1 (T)
	Elective Course (P) – 5 [EC (P)-5]	5	5 (L) + 1 (T)
	Project	5	10

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

Full Marks: 70+30
Total Lecture: 70 Hours

Eight questions are to be set out of which five are to be answered.

I Nature of Bonding in Main Group Inorganic Compounds 15 Hrs

VSEPR, Chemical Bonding- VSEPR model, Walsh diagrams (tri-atomic molecules of type AH_2), $d\pi-p\pi$ bonds, shapes of molecules- ClF_3 , ICl_4^- , TeF_5^- , I_3^- , $TeCl_6^{2-}$, XeF_6 , $SbCl_6^{3-}$, IF_7 , ReF_7 ; Bent rules and energetics of hybridization; electronegativity and partial ionic character; Some simple reactions of covalently bonded molecules, Atomic Inversion, Berry Pseudorotation. Bonds-Multicenter, Synergic and Agostic bonding. Lattice energy: Born-Landé equation, Kapustinskii equation; polarizability and partial covalent character, radius-ratio rules, structures of simple solids, Zintl-isoelectronic relationship in solids. Molecular orbital theory: MO diagrams of heteronuclear diatomic (CO and NO).

II Crystal Structure of Ionic Compounds 15 Hrs

Ionic crystals and their structures, radius ratio rule, effect of polarization on crystals. Covalent structure type- Sphalerite & Wurtzite, Geometry of simple crystal AB type: NaCl, CsCl & NiAs, reasons for preference for a particular structure in above AB type of compounds. AB_2 type: Fluorite, antiferrofluorites, Rutile structures. Li_2O , Na_2O , $CdCl_2$, CdI_2 structures. Defects in Solids: Point defects, Line defects and Plane defects. Ternary Compounds ABO_3 type: Perovskite, Barium titanate, lead titanate, $CaTiO_3$, $FeTiO_3$, Tolerance factor, charge neutrality and deviation structures. AB_2O_4 type-compounds: Normal & inverse, 2-3 and 4-2 spinel, site preferences in spinel, distorted spinel, Factors causing distortion in spinel.

III Unifying Principles 10 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.

IV Surface Chemistry 20 Hrs

Surface chemistry, types of adsorption curves, experimental methods of determining adsorption, Freundlich adsorption isotherm and its derivation, Traube's rule, Langmuir adsorption isotherm and its derivation, BET isotherm for multilayers and its derivation, properties of BET equation, methods for Determining surface area, heat of adsorption and its calculation, entropy of adsorption, Polanyi's potential theory, statistical treatment of Langmuir's adsorption isotherm, kinetics of gaseous reactions on solid surface: unimolecular and bimolecular surface reaction, temperature dependence of surface

reactions, electrocapillarity, electrokinetic effects. Gibb's adsorption equation and its derivation, verification of Gibb's adsorption equation, surface excess.

V Nuclear Chemistry

10 Hrs

Nuclear Chemistry-The atomic nucleus-elementary particles, quarks, classification of nuclides based on Z and N values, nuclear stability, nuclear potential, binding energy. Nuclear Models: Shell model-salient features, forms of the nuclear potential, filling of orbitals, nuclear configuration, Liquid drop model, Fermi gas model, Collective model and Optical model. Radioactivity, radioactive decay kinetics, Parent-daughter decay-growth relationship-secular and transient equilibria, theories of α , β^- , β^+ and γ -decay, internal conversion, Auger effect.

Reference Books

1. Inorganic Chemistry IV edition; J. E. Huheey, E. A. Keiter and R. L. Keiter, Addison; Wesley (1993).
2. Advanced Inorganic Chemistry, 6th edition; F. A. Cotton and G. Wilkinson.
3. Inorganic Chemistry, II edition, D. F. Shriver, P. W. Atkins and C. H. Langford, ELBS; Oxford University Press, 1994.
4. Concise Inorganic Chemistry, 5th edition; J. D. Lee (1996).
5. Physical Chemistry- Waller J. Moore
6. Physical Chemistry - P.W. Atkins
7. Inorganic Chemistry, 3rd Edition; Gary. L. Miessler and Donald . A. Tarr (2007).
8. Essentials of Nuclear Chemistry, 4th edition; H. J. Arniker, NAIL publishers (1995); Chapters 1, 3 and 4.
9. Nuclear and Radioactive Chemistry: Friedlander, Kennedy and Miller; Chapters 8 and 9.
10. Solid State Chemistry, D.K. Chakraborty (New Age Int. Publication)
11. Physical Chemistry of Surfaces, A. W. Adamson, Interscience Publisher Inc., New York (1967).
12. Surface Chemistry: Theory and Applications, J. J. Bikerman, Academic Press. New York (1972).

M.Sc. Semester-II
Core Course – 1 (CC-1)
(Transition Metal Complexes)

Full Marks: 70+30
Total Lecturer: 70 Hours

Eight questions are to be set out of which five are to be answered.

I Reaction Mechanism of Transition Metal Complexes 25 Hrs

- (A) Energy profile of a reaction, reactivity of metal complexes, Reaction mechanism- Labile, inert, stable and unstable complexes. Classification of mechanisms - Energy profile of reactions having different mechanisms. Kinetic application of valence bond and crystal field theories, Kinetics of octahedral substitution, 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 - Factors affecting substitution, Reactivity of Platinum complexes: Influences of entering and leaving groups, Trans effect in the synthesis of complexes, Theories of trans-effect, Application of trans-effect in the synthesis of complexes. Mechanism of ligand substitution in octahedral complexes: Kinetics and Factors affecting substitution in octahedral complexes: Leaving group, Chelate and Metal effects. Redox reactions.
- (B) Acid-Base catalysis: Acid catalysed aquation and anation reactions, acid hydrolysis, base hydrolysis, conjugate base hydrolysis, mechanism of acid hydrolysis and base hydrolysis stereochemistry of octahedral substitution, Replacement of coordinated water - Conjugate base mechanism, evidences in favour of the mechanism, application in the synthesis of platinum and cobalt complexes.
- (C) Electron transfer reactions – Outer sphere electron transfer reaction, Marcus equation, Inner sphere electron transfer reaction, formation and rearrangement of precursor complexes, the bridging ligand, successor complexes, cross reactions and Marcus-Hush theory. Use of electron transfer reactions for the synthesis of complexes.

II Stereochemistry of Transition Metals Complexes 10 Hrs

Stereochemical aspects - Stereoisomerism in inorganic complexes, isomerism arising out of ligand distribution and ligand conformation, chirality and nomenclature of chiral complexes.

III Stability of Transition Metals Complexes 10 Hrs

Stability of complexes - Factors affecting stability of complexes, thermodynamic aspects of complex formation, Stepwise and overall formation constants, stability correlations, statistical and chelate effects, Determination of stability constant - Polarographic, photometric and potentiometric methods.

IV Electronic Spectra of Transition Metal Complexes 15 Hrs

Spectroscopic ground states, selection rules, term symbols for d^n ions, Racah parameters, Orgel, Correlation and Tanabe-Sugano diagrams for transition metal complexes (d^1 - d^9)

states). Spectra of 3d metal-aqua complexes of trivalent (V and Cr), divalent (Mn, Co and Ni) complexes and CoCl_4^{2-} . 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. Spectral properties of Lanthanide and Actinide metal complexes.

V Magnetic Properties of Transition Metal Complexes

10 Hrs

Magnetic properties of coordination compounds - Types of magnetic behaviour, magnetic susceptibility and its determination : Gouy, Faraday, and VSM method. Diamagnetic correction, orbital contribution, spin-orbital coupling, ferro- and antiferro- magnetic coupling, magnetic exchange coupling and spin-crossover. Anomalous magnetic moments and their explanation. Magnetic properties of Lanthanide and Actinide metal complexes.

Reference Books

1. Inorganic Chemistry IV edition; J. E. Huheey, E. A. Keiter and R. L. Keiter, Addison; Wesley (1993).
2. Advanced Inorganic Chemistry, 6th edition; F. A. Cotton and G. Wilkinson.
3. Inorganic Chemistry, II edition, D. F. Shriver, P. W. Atkins and C. H. Langford, ELBS; Oxford University Press, 1994.
4. Concise Inorganic Chemistry, 5th edition; J. D. Lee (1996).
5. Inorganic Chemistry, 3rd Edition; Gary. L. Miessler and Donald . A. Tarr (2007).
6. Physical Methods in Chemistry, R.S. Drago, Saunders College.
7. Chemistry of the Elements, N.N. Greenwood and A. Earnshaw, Pergamon.
8. Inorganic Electron Spectroscopy, A. B. P. Lever, Elsevier (1968)
9. Magnetochemistry, R.L. Carlin, Springer Verlag,
10. Electronic Absorption Spectroscopy and Related Techniques, D. N. Sathyanarayana, University Press (2001).
- 11 Comprehensive Coordination Chemistry eds., Q. Wilkinson, R.D. Gillars and J.A. McCleverty, Pergamon.

M.Sc. Semester-I
Core Course – 2 (CC-2)
(Reaction Mechanism in Organic Chemistry)

Full Marks: 70+30
Total Lecture: 70 Hours

Eight questions are to be set out of which five are to be answered.

I Nature of Bonding in Organic Molecules 15 Hrs

Aromaticity in benzenoid and non-benzenoid compounds(including annulenes and heterocyclic compounds), alternant and non-alternant hydrocarbons, Huckel's rule, energy level of π -molecular orbitals, azulene, annulenes, anti-aromaticity, π - aromaticity, homo-aromaticity, PMO approach.

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

II Stereochemistry 15 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 activity, 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. Regioselectivity.

III Aliphatic Nucleophilic Substitution 10 Hrs

The S_N2 , S_N1 , mixed S_N1 and S_N2 and SET mechanisms. The neighbouring group mechanism, neighbouring group participation, anchimeric assistance.

Classical and nonclassical carbocations, phenonium ions, norbornyl system, common carbocation rearrangements.

The S_Ni 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.

IV Aromatic Nucleophilic Substitution 05 Hrs

The S_{NAr} , S_{NO} , benzyne and S_{RO} mechanisms. Reactivity - effect of substrate structure, leaving group and attacking nucleophile. The von Richter, Sommelet-Hauser, and Smiles rearrangements.

V Aliphatic Electrophilic Substitution 05 Hrs

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

VI Aromatic Electrophilic Substitution 10 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. Diazo-coupling reaction, Vilsmeier reaction, Gattermann-Koch reaction.

VII Free Radical Reactions

10 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. Reactivity 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.

Reference Books

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. Pericyclic Reactions, S. M. Mukherji, Macmillan, India.
7. Reaction Mechanism in Organic Chemistry, S. M. Mukherji and S. P. Singh, Macmillan.
8. Stereochemistry of Organic Compounds, D. Nasipuri, New Age international.

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

Full Marks: 100

Pass Marks: 50

Time: 06 Hrs

Two questions are to be set.

I Estimation of the following

- (i) Magnesium by EDTA (Volumetrically)
- (ii) Zinc by Potassium ferrocyanide (Volumetrically)
- (iii) Nickel by Dimethylglyoxime (Gravimetrically)
- (iv) Manganese in steel by Sodium bismuthate method.

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

- (i) Preparation of Methyl Orange
- (ii) Preparation of Martius yellow
- (iii) Preparation of p-Nitro aniline from Acetanilide
- (iv) Preparation of Cinnamic acid from Benzaldehyde

III Estimation of

- (i) Glucose using Fehling's solution
- (ii) Carbonyl group using 2,4-Dinitrophenyl hydrazine

Practical-1: 40 Marks, Practical-2: 40 Marks, Note Book: 10 Marks, Viva: 10 Marks.

M.Sc. Semester-II
Elective Course (SE) (EC-1)
Introduction to Computers for Chemist

Full Marks: 70+30
Total Lecture :70 Hours

Eight questions are to be set out of which five are to be answered.

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 Huckel 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
Biochemistry

Full Marks: 70+30
Total Lecturer: 70 Hours

Eight questions are to be set out of which five are to be answered selecting at least one question from each group.

Group A: Biophysical Chemistry

I Bioenergetics 10 Hrs

Standard free energy, entropy and chemical potential change in biochemical reactions. The effect of temperature and pH on ΔG° . Methods of determination of free energy changes. Relationship between K_{eq} and ΔG° . Oxidation, reduction reaction and hydrolytic reactions in biological system, redox potential (electron-transfer reactions), free energy changes of oxidation-reduction reactions.

II Enzymes and Mechanism of Enzyme Action 15 Hrs

Basic considerations. Proximity effects and molecular adaptation. Enzymes : 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 Koshland'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.

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.

Group B: Bioinorganic Chemistry

III Essential and trace metals ions in biological systems 15 Hrs

Biological functions of inorganic elements, biological ligands for metal ions. Coordination by proteins, Tetrapyrrole ligands and other macrocycle. Influence of excess and deficiency of V, Cr, Mn, Fe, Co, Cu, & Zn. Genetic defects in the absorption of trace elements. Regulation and storage of trace elements. Role of minerals. Toxic effects of metals.

Metal storage, transport and biomineralization with respect to Ferritin, Transferrin and Siderophores, Na^+ / K^+ pump. Role of Ca in transport and regulation in living cells.

Medicinal use of metal complexes as antibacterial, anticancer, use of cis-platin as antitumor drug, antibiotics & related compounds. Metal used for diagnosis and chemotherapy with particular reference to anti cancer drugs.

IV Bioenergetics and Biochemistry of Dioxygen 10 Hrs

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

Oxygen transport and oxygen uptake proteins- transport and storage of dioxygen, Heme proteins and oxygen uptake, Non-porphyrin systems-hemerythrin and hemocyanin, dioxygen binding, Structure and function of hemoglobin, myoglobin, hemocyanins and hemerythrin, Bohr effect, Hill equation, Perutz mechanism showing structural changes in porphyrin ring system. Oxygenation and deoxygenation. Role of distal and proximal histidine; Model complexes for dioxygen binding. Synthetic complexes of iron, cobalt and copper. Cyanide poisoning and treatment. Vanadium storage and transport.

Group C: Bioorganic Chemistry

V Kinds of Reactions Catalysed by Enzymes **10 Hrs**
Nucleophilic displacement on a phosphorus atom, multiple displacement reactions and the coupling of ATP cleavage to endergonic processes. Mechanisms for phosphoryl transfer reactions, The mechanistic role of the coenzymes in living systems : (i) Biotin coenzyme in carboxylation reactions, (ii) Thiamine pyrophosphate (TPP) in decarboxylation, (iii) Coenzyme A (CoASH) in the transfer of acyl group, (iv) Vitamin B₁₂ coenzymes in molecular rearrangement reactions and in the synthesis of methionine and methane.

VI Co-Enzyme Chemistry **10 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, lipolic acid, vitamin B₁₂. Mechanisms of reactions catalyzed by the above cofactors.

Reference Books

1. Introduction to Biophysical chemistry, R. Bruce Martin, McGraw-Hill, NY, 1964.
2. Physical Chemistry with applications to Biological systems, Ramond Chnag, Mc Millan publishing Co.inc, New York 1977.
3. Understanding Enzymes, Trevor Palmer, Prentice Hall.
4. Enzyme Chemistry: Impact and Applications, Ed. Collin J Suckling, Chapman and Hail.
5. Enzyme Mechanisms Ed, M. I. Page and A. Williams, Royal Society of Chemistry.
6. Enzymatic Reaction Mechanisms, C. Walsh, W. H. Freeman.
7. Enzyme Structure and Mechanism, A Fersht, W.H. Freeman.
8. Biochemistry: The Chemical Reactions of Living Cells, D. E. MeUler, Academic Press.
9. Principles of Bioinorganic Chemistry, S.J. Lippard and J.M. Berg, University Science Books.
10. Bioinorganic Chemistry, I. Bertini, H.B. Gray, S.J. Lippard and J.S. Valentine, University Science Books.
11. Bioorganic Chemistry: A Chemical Approach to Enzyme Action, Hermann Dugas and C. Penny, Springer-Verlag.

2. Inorganic Photochemistry, Fmiza Hammer, Sarup Book Publishers Pvt. Ltd., New Delhi.
3. Concepts of Inorganic photochemistry, A. W. Adamson and P D Fleischaves Wiley.
4. Elements of Inorganic Photochemistry G. J. Ferranti, Wiley.
5. Progress in Inorganic Chemistry, Vols 18 and 38 ed. J.J. Lippard, Wiley.

OR
Physical Organic Chemistry

Full Marks: 70+30
Total Lecture: 70 Hours

Eight questions are to be set out of which five are to be answered.

- I Reaction Mechanism: Structure and Reactivity** **10 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. Theory of isotope effects: Primary and secondary kinetic isotope effects. Heavy atom isotope effects. Tunneling effect. Solvent isotope effects. Effect of structure on reactivity resonance and field effects, Steric effect, quantitative treatment, The transition state theory of isotope effects.
- II Concepts in Molecular Orbital Theory** **10 Hrs**
- Introduction to Huckel molecular orbital (MO) method as a means to explain modern theoretical methods. Qualitative MO theory - Ionisation potential, Electron density. MO energy levels. Orbital symmetry. Orbital interaction diagrams. Huckel theory of conjugated systems: Applications to ethylene, propeny system, cyclopropenyl system, butadiene and cyclobutadiene, bond order and charge density calculations.
- III Steric and Conformational Properties** **15 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.
- IV Structural Effects on Reactivity** **15 Hrs**
- Linear free energy relationships (LFER). The Hammett equation, Substituent constants, Theories of substituent effects. Taft model, σ_{meta} - and σ_{para} -, σ^+ and σ^- constants, Polar and Steric substituent constants in aliphatic systems, Dual-parameter substituent constant,
- V Principles of Reactivity** **20 Hrs**
- Mechanistic significance of entropy, enthalpy and Gibb's free energy, solvent polarity scales. Kinetics and Mechanism : The rate equations, first order kinetics through constant concentration of a reagent, kinetic and thermodynamic control, complex systems, The Arrhenius equation, Transition state theory, potential energy surface, The reaction coordinate, Hammond's postulate and its experimental support, Three dimensional reaction

coordinate diagrams, Valence bond model, Marcus reaction rate theory, Bell-Evans-Polanyi principle. Potential energy surface model. Electron transfer reactions and theories. Reactivity and selectivity principles.

Reference Books

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. The Physical Basis of Organic Chemistry, H. Maskill, Oxford University Press.

OR

Statistical Thermodynamics and Surface Chemistry

Full Marks: 70+30

Total Lecture: 70 Hours

Eight questions are to be set out of which five are to be answered.

I Statistical Thermodynamics

15 Hrs

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 Lagrange's method of undetermined multipliers). Partition functions-translational, rotational, vibrational and electronic partition functions. Applications of partition functions, Fermi-Dirac statistics, distribution law and applications to metal. Bose-Einstein statistics. Distribution law and its application to helium.

II Potential Energy Surfaces

10 Hrs

Mechanism of activation, Potential energy surface for three atom reaction, Potential energy curve for successive reactions, Properties of potential energy surfaces, Inter conversion of translational and vibrational energies, Combination of atoms, Ortho-para conversion, Activated state of three atom and four atom reactions, Potential energy profile, reaction coordinate, Transmission co-efficient, non-adiabatic reaction.

III Kinetics of condensed phase reactions

10 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 contribution to free energy in single and double spherical models of activated complex, 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.

IV Study of Fast Reactions

10 Hrs

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

V Surface Chemistry

25 Hrs

- A. Adsorption** : Surface tension, capillary action, pressure difference across curved surface (Laplace equation), Vapour pressure of droplets (Kelvin equation), Classical and modern methods for determining surface structure and composition, Surface films on liquids (Electro-kinetic phenomena), criteria for spreading of one liquid on another, Surface pressure and measurement of surface pressure, Langmuir surface balance and molecular dimensions, states of mononuclear films, reaction in monomolecular films , types and structure of surface films: optical method, electrical method.
- B. Micelles** : Surface active agents, classification of surface active agents, micellization, hydrophobic interaction, critical micellar concentration (CMC), factors affecting the CMC of surfactants, counter ion binding to micelles, thermodynamics micellization-phase separation and mass action models, solubilization, micro emulsion, reverse micelles.
- C. 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.

Reference Books

1. Physical Chemistry- Waller J. Moore
2. Physical Chemistry - P.W. Atkins, ELBS.
3. Principles of polymer chemistry Cornell , P. J. Flory (Univ. Press)
4. Handbook of Conducting Polymers Vol I & II" T A. Skolhia.
5. Introduction to Quantum Chemistry, A.K. Chandra, Tata McGraw Hill.
6. Quantum Chemistry, Ira N. Levine, Prentice Hall.
7. Coulson's Valence, R. McWeeny, ELBS.
8. Chemical Kinetics, K. J. Laidler, Mcgraw-Hill.
9. Kinetics and Mechanism of Chemical Transformations, J. Rajaraman and J. Kuriacose, McMillan.
10. Modern Electrochemistry Vol. I and Vol. II, J.O.M. Bockris and A.K.N. Reddy, Plenum.
11. Introduction to Polymer Science, V.R. Gowarikar, N.V. Vishwanathan and J. Sridhar, Wiley Eastern.

M.Sc. Semester-II
Core Course – 4 (CC-4)
(Quantum Chemistry and Chemical Dynamics)

Full Marks: 70+30
Total Lecturer: 70 Hours

Eight questions are to be set out of which five are to be answered.

I. Quantum Chemistry

35 Hrs

A. Introduction to Exact Quantum Mechanical Results

Concept of operator, 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 Hydrogen atom.

C. Qualitative treatment of hydrogen atom

Setting up of Schrödinger equation in spherical polar coordinates, radial part, quantization of energy (only final energy expression).

D. Chemical bonding

Covalent bonding, valence bond and molecular orbital approaches, LCAO-MO treatment of H_2^+ . Bonding and antibonding orbitals. Qualitative extension to H_2 . Comparison of LCAO-MO and VB treatments of H_2 (only wavefunctions, detailed solution not required) and their limitations. Refinements of the two approaches (Configuration Interaction for MO, ionic terms in VB). Qualitative description of LCAO-MO treatment of homonuclear and heteronuclear diatomic molecules (HF, LiH). Localised and non-localised molecular orbitals treatment of triatomic (BeH_2 , H_2O) molecules. Qualitative MO theory and its application to AH_2 type molecules.

E. Angular Momentum

Ordinary angular momentum, generalized angular momentum, eigen-functions for angular momentum, eigen-values of angular momentum, operator using ladder operators, addition of angular momenta, spin, antisymmetry and Pauli exclusion principle.

F. Electronic Structure of Atoms

Electronic configuration, Russell-Saunders terms and coupling schemes, Slater-Condon parameters, term separation energies of the p^n 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.

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 Duhem equation, Nernst heat theorem and its applications, Determination of absolute entropy, Maxwell's thermodynamic relation.

III Chemical Dynamics

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. 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).

Reference Books

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

M.Sc. Semester-II
Core Course – 5 (CC-5)
(Group Theory and Spectroscopy)

Full Marks: 70+30
Total Lecture: 70 Hours

Eight questions are to be set out of which five are to be answered.

- I Symmetry and Group Theory in Chemistry** **25 Hrs**
- Symmetry elements and symmetry operation, Group and Subgroup, Point group, Classification and representation of groups, The defining property of a group, Sub group and Class, Group multiplication table for C_{2V} , C_{2h} and C_{3V} point group, Generators and Cyclic groups. Similarity Transformation, Table of conjugates for C_{2V} , C_{2h} and C_{3V} point group, Schonflies symbols.
- Matrix notation for symmetry operation, Representations of groups by matrices (representation for the C_n , C_{nv} , C_{nh} and D_{nh} groups to be worked out explicitly). Character of a representation, Mulliken symbols for irreducible representations, Direct product relationship, Applications of group theory to quantum mechanics-identifying non-zero matrix elements.
- The great orthogonal theorem (without proof) and rules derived from this theorem. Derivation of the orthonormalization condition. Character table. Construction of character table: C_{2V} and C_{3V} (only). Reducible representations and their reduction. Application of character table in determination of IR and Raman active vibrations in H_2O , BF_3 and N_2F_2 .
- II Microwave Spectroscopy** **10 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.
- III Vibrational Spectroscopy** **15 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).
- IV 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.

V Mass Spectrometry

10 Hrs

Basic principles - Ion production : Soft ionization methods, Low energy electron ejection, Chemical ionization, Ionization of large molecules : Fast-atom bombardment (FAB), Plasma desorption (PD) and Matrix Assisted Laser Desorption/ionization (MALDI), Electrospray ionization (ESI), Pyrolysis, Exact mass measurements, Tandem mass spectrometry. Quadrapole mass spectrometers: FT-ICR

Reference Books

1. F. A. Cotton, Chemical Application of Group Theory , John wiley and Sons Inc.,Newyork, 1971.
2. N. Tinkham, Group Theory and Quantum Mechanics , McGraw Hill Book Company, Newyork, 1964.
3. Alan Vincent, Molecular Symmetry and Group theory – Programmed Introduction to chemical applications , Wiley, Newyork, 1977.
4. Physical Methods for Chemistry, R.S. Drago, Saunders Company.
5. Modern Spectroscopy, J.M. Hollas, John Wiley.
6. Physical Methods in Chemistry, R.S. Drago, Saunders College.
7. Introduction to Molecular Spectroscopy, Q.M. Barrow, McCraw Hill.
8. Basic Principles of Spectroscopy. R. Chang, McGraw Hill.
9. Theory and Applications of UV Spectroscopy, H.H. Jatie and M. Orehin, IBH-Oxford.
10. Introduction to Magnetic Resonance, A. Carrington and A.D. Maclachalan, Harper & Row.
11. Structural Methods in Inorganic Chemistry, E.A.V. Ebsworth, D.W.H. Rankin and S. Cradock, ELBS
12. Infrared and Raman Spectra: Inorganic and Coordination Compounds, K. Nakamoto, Wiley.
13. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R.V. Parish, Ellis Horwood.
14. Vibrational Spectroscopy: Theory and Applications, D. N. Sathyanarayana, New Age Publications.
15. Introduction to Molecular Spectroscopy, C. N. Banwell, TMH Edition.

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

Full Marks: 100

Pass Marks: 50

Time: 06 Hrs

Two questions are to be set.

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_3COOH).
- (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

Determination of partition coefficient of:

- (i) Benzoic acid between water and Benzene
- (ii) Iodine between water and carbon tetrachloride

8. Estimation of following in the supplied water,

Ca, Iron, Lead, Mg, Nitrate, Chloride

9. Estimation of following in the supplied soil sample,

Ca, Mg, Carbonate carbon, Organic matter, Total nitrogen, Ammonia, Nitrate nitrogen

Practical-1: 40 Marks, Practical-2: 40 Marks, Note Book: 10 Marks, Viva: 10 Marks.

M.Sc. Semester-III
Core Course – 7 (CC-7)
Application of Spectroscopy

Full Marks: 70+30
Total Lecture: 70 Hours

Eight questions are to be set out of which five are to be answered.

I Ultraviolet and Visible Spectroscopy 10 Hrs

Types of electronic transitions (185-800 nm), Beer-Lambert law, Effect of solvent polarity on electronic transitions, Chromophores and Auxochromes, Absorption and Intensity shift; Bathochromic, Hypsochromic shifts, Hyperchromic and Hypochromic shifts. Application of Fieser-Woodward Rules for calculation of λ_{\max} for Conjugated dienes: alicyclic, homoannular, heteroannular, extended conjugated systems (aldehydes, ketones and dienes), Distinction between cis and trans isomers. Application of Fieser-Woodward Rules for calculation of λ_{\max} for the following systems: α , β - unsaturated aldehydes, ketones, carboxylic acids and esters. Ultraviolet and visible spectra of aromatic and heterocyclic compounds.

II Infrared Spectroscopy 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 carbonyl compounds (ketones, aldehydes, esters, amides, acids, anhydrides, lactones, lactams and conjugated carbonyl compounds). Effect of hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination bands and Fermi resonance. FTIR. IR of gaseous, solids and polymeric materials.

III Nuclear Magnetic Resonance Spectroscopy 15 Hrs

Basic principle of PMR Spectroscopy, chemical shift, spin-spin coupling and coupling constant, Pascal's triangle-low and high resolution, reference compounds (internal and external), nuclear shielding and deshielding phenomenon, chemical shift and factors influencing it, Anisotropic effects in alkene, alkyne, aldehydes, acids and aromatics. Chemical shift correlation for protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic) and other nuclei (alcohols, phenols, enols, carboxylic acids, amines and amides), chemical exchange, effect of deuteration, solvent effects. Fourier transform technique. Interpretation of PMR spectra of simple organic compounds (such as ethyl bromide, ethanol, 1,1,2-tribromoethane, acetaldehyde, acetic acid and ethyl acetate).

¹³C-NMR Spectroscopy 05 Hrs

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

IV Mass Spectrometry 10 Hrs

Introduction, ion production - EI, CI, FD and FAB, factors affecting fragmentation, ion analysis, ion abundance. Mass spectral fragmentation of organic compounds : alkanes, alkenes, alkyl halides, alcohols, aldehydes, ketones (cyclic and acyclic compounds), acids, esters, ethers, amines, nitro compounds, halo compounds and peptides. Factors affecting

cleavage patterns. Molecular ion peak, Metastable peak, McLafferty rearrangement. Nitrogen rule. High resolution mass spectrometry. Examples of mass spectral fragmentation of organic compounds with respect to their structure determination. Use of HRMS to determine exact molecular weight of compounds

V Electron Spin Resonance Spectroscopy 10 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 to five unpaired electrons) including biological systems and to inorganic free radicals such as PH_4 , F_2^- and $[\text{BH}_3]^-$.

VI Mössbauer Spectroscopy 10 Hrs

Basic principles, Isomer shift, Quadrupole splitting and Magnetic hyperfine interactions. 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.

Reference Books

1. Organic Spectroscopy, P. Laszlo and P. Strang, Harper and Row, New York, 1971.
2. Organic Spectroscopy, W. Kemp, ELBS London, 2000.
3. Introduction to Spectroscopy, 3rd Edition, D. L. Pavia, G. M. Laupman and G. S. Kriz, Harcourt college publishers.
4. Interpretation of Mass Spectra, 4th edition, F.W. McLafferty, F. Turecek, California
5. Practical Organic Mass Spectroscopy, 2nd edition, J. R. Chapman, John Wiley, NY, 1993,
6. The IR spectra of complex molecules, Vols.1 and 2, L. J. Bellamy, Chapman and Hall, London
7. Spectroscopic Techniques for Organic Chemists, J. W. Cooper, John Wiley, NY
8. Bimolecular NMR Spectroscopy, J N S Evans, Oxford univ. 1995.
9. Mass Spectroscopy A Foundation Course. K. Downard, RSC, Cambridge.
10. Instrumental Methods of Analysis, H. H. Willard, L. L. Merrit, J. A. Dean and F.A.Settle, CBS Publishers and Distributors
11. Practical NMR Spectroscopy, M.L Martin, J.J. Delpuech and Q.J.F Artin, Heyden.
12. Spectrometric Identification of Organic Compounds, R. M. Silverstein, Q. C. gassier and T. C. Morrill, John Wiley
13. Application of Spectroscopy of Organic Compounds, J. R. Dyer, Prentice Hail.
14. Spectroscopic Methods in Organic Chemistry, D. H. Williams, I. Fleming, Tala McGraw Hill.
15. Vibrational Spectroscopy: Theory and Applications, D. N. Sathyanaarayana, New Age Publications.

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

Full Marks: 70+30
Total Lecture: 70 Hours

Eight questions are to be set out of which five are to be answered.

I Environment and Atmosphere 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 O. Biodistribution of elements. 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, chlorofluorohydrocarbons. Green house effect, acid rain, air pollution controls and their chemistry. Analytical methods for measuring air pollutants. Continuous monitoring instruments.

II Hydrosphere 10 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, Pollutants-fertilizers, pesticides, plastics and metals. Waste treatment.

IV Industrial Pollution 05 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.

V Environmental Toxicology 10 Hrs

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

VI Analysis of Water Pollution 10 Hrs

Origin of waste water, types, water pollutants and their effects. Sources of water pollution-domestic, 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.

VII Analysis of Soil, Food, Fuel, Body Fluids and Drugs

20 Hrs

- (a) Analysis of soil: moisture, p^H , total nitrogen, phosphorus, silica, lime, magnesia, manganese, sulphur and alkali salts.
- (b) Food Analysis: Moisture, ash, crude protein, fat, crude fiber, 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.
- (c) Fuel analysis: solid, liquid and gas. Ultimate and proximate analysis-heating values - grading of coal. Liquid fuels-flash point, aniline point, octane number and carbon residue. Gaseous fuels-producer gas and water gas-calorific value.
- (d) 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 analysis of trace elements in the body.
- (e) Drug analysis: Narcotics and dangerous drugs. Classification of drugs. Screening by gas and thin-layer chromatography and spectrophotometric measurements.

Reference Books

1. Environmental Chemistry, S. E. Manahan, Lewis Publishers.
2. Environmental Chemistry, Sharma & Kaur, Krishna Pabilshers.
3. Environmental Chemistry, A. K. De, Wiley Easlem.
4. Environmental Pollution Analysis, S.M. Khopkar, Wiley Eastern
5. Environmental Toxicology, Ed. J. Rose, Gordon and Breach Science Publication.
6. Elemental Analysis of Airborne Particles, Ed. S. Landsberger and M. Crealchman, Gordon and Breach Science Publication.
7. Environmental Chemistry, C. Baird, W. H. Freeman.
8. Handbook of Instrumental Techniques for Analytical Chemistry, F. Settle, Prentice Hall.
9. Fundamentals of Analytical Chemistry, D.A. Skoog, D.M. West and F.J. Holler, W. B. Saunders.

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

Full Marks: 70+30
Total Lecture: 70 Hours

Eight questions are to be set out of which five are to be answered.

I Organotransition Metal Complexes 15 Hrs

Chemistry of Organotransition metal complexes: General introduction. 18- and 16-Electron rules. General rules. Complexation and De-complexation Reactions: s-Bonded systems including η^1 ligands. p-Bonded systems involving dihapto to octahapto ligands such as- olefins, acetylenes, allyl moieties, butadiene, cyclobutadiene, arenes, cyclopenta, cyclohexa and cycloheptadienyl moieties; cyclohepta, cyclooctatrienes, and cyclooctatetraene moieties.

Use of organotransition metal complexes as protecting and stabilizing groups: Protection of olefins, acetylenes and dienes. Stabilization of cyclobutadienes and norbornadienones. Organometallics as electrophiles and nucleophiles: Nucleophilic addition to η^2 , η^5 and η^6 complexes. Electrophilic addition to η^4 , η^6 and carbene complexes.

II Organometallic Compounds in Synthesis-II 15 Hrs

Organometallics in coupling and cyclization reactions: Coupling and cyclization of organic nucleophiles with olefins (including Heck reaction), and coupling of olefins with acetylenes (including Felkin's reaction).

Organometallics in isomerization, oxidation and reduction reactions: Isomerization of olefins, allylic alcohols and allylic ethers. Oxidation of olefins (including Wacker's process and epoxidation) and reduction of olefins and α,β -unsaturated compounds (including Wilkinson's reaction).

III Organometallic Compounds in Synthesis-III 30 Hrs

(Organozincs, Organolithiums, Organocopper, Organoseleniums, Organotelluriums, Organoaluminiums, Use of zirconium, iron, cobalt and palladium complexes.)

Application of the following organometallics in synthesis: Organozincs: Preparation, reaction with compounds containing acidic protons, reaction with C-C multiple bonds, trans-metallation, addition reactions of zinc reagents with carbonyl compounds. Organolithiums: Preparation. Deprotonation reactions, nucleophilic addition reactions, reactions with imines, nitriles and isonitriles. Organocopper reagents: (Gilman reagents-lithium dialkyl cuprates): Preparation, reactions with alkyl, allyl, vinyl, benzyl and aryl halides, aldehydes, ketones (including α,β -unsaturated carbonyl compounds) and epoxides.

Organoseleniums: Preparation, use of organoseleniums in the synthesis of alkenes, α,β -unsaturated carbonyl compounds. Organotelluriums: Debromination of vic-dibromides, deoxygenation of epoxides, oxidation of hydroquinone and synthesis of biaryls. Organoaluminiums: Preparation, hydroalumination and carboalumination of alkenes.

Nucleophilic addition reactions with carbonyl compounds and Hydrocyanation. Preparation of alkenyldialkylalanes and their reactions.

Carbonylation reactions: Use of zirconium complexes in the synthesis of esters, acids, aldehydes, acyl halides and in the hydroformylation of olefins and dienes. Use of iron complexes for the insertion of CO group. Use of cobalt complexes in the synthesis of ketones from epoxides, lactones from allylic alcohols and in the hydroformylation of olefins. Use of palladium complexes for the carbonylation of alkyl halides, dienes and allenes.

IV Organometallic compounds in synthesis-IV **10 Hrs**
(Organosilicons, Organotin, Organocerates, and Organomercurials)

Organosilicons: Introduction, preparation and general reactions of trialkylsilyl halides. Peterson olefination. Organotin: Preparation and reactions of tri-n-butyltin hydride, Barton decarboxylation and Barton-McCombie reaction. Organocerates: Preparation and reactions of organocerates. Organomercurials: Preparation. Electrophilic substitution reactions. Solvomercuration-demercuration and cyclopropanation of alkenes.

Reference Books

1. The Organometallic Chemistry of the transition metals, R. H. Crabtree, 1988.
2. Principles and application of the organotransition metal chemistry, J. P. Collman, L. S. Hege, University Science books, 1980.
3. Modern Synthetic Reactions, H. O. House, W.A. Benjamin, California, 2nd Edn. 1972.
4. Organometallics, Vol. 1 & 2, M. Bochmann, Oxford Chemistry primers, Oxford University Press, 1994.
5. Organotransition metal chemistry, S. G. Davies, Pergamon Press, Oxford, 1982.
6. Principles and Application of Organotransition Metal Chemistry, J.P. Collman, L.S. Hege, J.R. Norton and R.G. Pinke, University Science Books.
7. The Organometallic Chemistry of the Transition Metals, R.H. Crabtree, John Wiley
8. Metallo-organic Chemistry, A.J. Pearson, Wiley.
9. Organometallic Chemistry, R.C. Mehrotra and A. Singh, New Age International.

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

Full Marks: 70+30
Total Lecture: 70 Hours

Eight questions are to be set out of which five are to be answered.

- I Supramolecular Chemistry 20 Hrs**
- Bonds weaker than covalent: Ion-ion interaction, ion-dipole interaction, dipole-dipole interaction, Ionic bond, Covalent bond, Hydrogen bonding. Molecular recognition: Molecular receptors for different types of molecules substrates, Supramolecular reactivity and catalysis. Supramolecular devices : Oxa-Crown Ethers, Aza-Crown Ethers, Cryptands, Corands, Podands, Spherands and Hemispherands, Cyclophanes, Calixarenes, Cyclodextrines, Catananes, Rotaxanes. Supramolecular reactivity and catalysis: Supramolecules with chiral framework (introduction only), Generating molecular cleft for binding. Some example of self-assembly in supramolecular chemistry, Nanomaterials with supramolecular structure, Molecular devices: Photo-switchable devices.
- II Chemistry of Selected Name Reactions-I 10 Hrs**
- A study of the following name reactions: Dieckmann cyclization, Shapiro reaction, Stork enamine reaction, Barton reaction, Ene reactions, Sharpless asymmetric epoxidation, Bayer–Villiger oxidation, Robinson annulations, Michael addition, Mannich reaction, Simmons-Smith reaction, Hoffmann-Löffler-Freytag reaction, Beker-Venkatraman rearrangement (Few examples in each rearrangement are to be studied).
- III Chemistry of Selected Name Reactions-II 10 Hrs**
- Darzen's reaction, Acid-catalyzed self condensation of olefins, Prins reaction, Hofmann-Martius reaction. Acyloin condensation. Meyer synthesis. Chichibabin reaction, Mitsunobu reaction, N-Nitroaromatic amine rearrangement, Fisher-Hepp reaction. Japp-Klingemann reaction (Few examples in each rearrangement are to be studied).
- IV Rearrangement Reactions 10 hour**
- Formation and stability of carbonium ions, carbanion, carbenes, nitrenes, radicals and arynes. Rearrangement involving carbonium ions: Wagner-Meerwein, Pinacol-Pinacolone rearrangement, reaction involving acyl cation, and Fries rearrangement, Rearrangement involving carbenes: Wolff & Arndst-Eistert synthesis. Rearrangement involving nitrenes: Hoffman, Curtius, Schmidt, Lossen and Beckman rearrangement.
- V Cross Coupling Reactions 10 Hrs**

The Suzuki-Miyaura reaction, The Heck reaction, Kumada reaction, Nozaki-Hiyama-Kishi reaction and Buchwald-Hartwig reaction.

VI Biomolecular Spectroscopy

10 Hrs

ORD – CD: Linearly and circularly polarized light, Circular birefringence and circular dichroism, ORD and CD curves, Cotton effect, Comparison of ORD and CD: Use of plain curves, Application of CD and ORD curves showing Single and Multiple Cotton effects : (i) Functional group analysis, (ii) Position of a functional group, (ii) Determination of configuration, and (iv) Study of conformational change, Axial haloketone rule, Octant rule for ketones and its application.

Reference Books

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.

function for electrons in solids, metallic conductors, insulator, semiconductors (intrinsic & extrinsic), properties of junctions, energy levels in extended, repeat and reduced zone schemes.

VI Electrical and Magnetic Properties of Solids

10 Hrs

Metals: calculation of density of states, origin of resistivity, weak paramagnetism
Semiconductors: Intrinsic and extrinsic- p and n-types, Hall effect, Junctions and their applications: metal-metal, metal-semiconductor, semiconductor-semiconductor types and transistors. Insulators - dielectric properties, piezo and inverse piezoelectric effects, ferroelectricity, ferroelectric transitions in BaTiO₃, ionic conductivity applications of band theory to TiO and NiO: Limitations of the Independent electron model, modeling electron correlation.

Reference Books

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. B. Hannay (Prentice Hall, New Jersey)
5. Physical Chemistry, P.W. Atkins
6. Principles of Polymer Chemistry, P. J. Flory (Univ. Press)
7. Handbook of Conducting Polymers Vol I & II", T A. Skolhia.

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

Full Marks: 100

Pass Marks: 50

Time : 06 Hrs

Two questions are to be set.

1. Qualitative separation and determination of the following pairs of metal ion using gravimetric and volumetric methods
 - a) $\text{Ag}^+(\text{g})$ and $\text{Cu}^{2+}(\text{v})$
 - b) $\text{Cu}^{2+}(\text{g})$ and $\text{Zn}^{2+}(\text{v})$
 - c) $\text{Fe}^{3+}(\text{g})$ and $\text{Ca}^{2+}(\text{v})$
 - d) $\text{Mg}^{2+}(\text{g})$ and $\text{Ca}^{2+}(\text{v})$
2. Semi micro qualitative analysis of a mixture containing five cations of rare element and insolubles.
 - 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
3. Gravimetric Analysis
 - a) Estimation of nickel (II) using Dimethylglyoxime (DMG)
 - b) Estimation of copper as CuSCN
 - c) Estimation of iron as Fe_2O_3 by precipitating iron as $\text{Fe}(\text{OH})_3$
 - d) Estimation of Al (III) by precipitating with oxine and weighing as $\text{Al}(\text{oxine})_3$
4. Inorganic Preparations
 - a) Cis and trans $\text{K}[\text{Cr}(\text{C}_2\text{O}_4)_2 \cdot (\text{H}_2\text{O})_2]$ Potassium dioxalatodiaquachromate (III)
 - b) Tetraamminecarbonatocobalt (III) ion
 - c) Potassium tris(oxalate)ferrate(III)
 - d) Tetraamminecopper (II) sulphate, $[\text{Cu}(\text{NH}_3)_4]\text{SO}_4 \cdot \text{H}_2\text{O}$

Practical-1: 40 Marks, Practical-2: 40 Marks, Note Book: 10 Marks, Viva: 10 Marks.

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

Full Marks: 100

Pass Marks: 50

Time : 06 Hrs

Two questions are to be set.

I Separation and Characterization of organic compounds from Binary systems:

- (i) liquid-liquid,
- (ii) liquid-solid
- (iii) solid-solid

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

- (i) Preparation of o-Chlorobenzoic Acid from Anthranilic acid
- (ii) Preparation of Iodobenzene from Aniline
- (iv) Preparation of p-Iodonitrobenzene from p-Nitroaniline
- (v) Anthraquinone from anthracene
- (vi) β -naphthyl methyl ether from β -naphthol

III Estimation:

- (a) To determine the percentage or number of phenolic groups in the given sample by The acetylation method.
- (b) To determine the percentage or number of methoxyl groups in the given sample by The Zeisel's method.
- (c) To determine the percentage or number of acetyl groups in an Acetyl Ester

IV Estimation of the amount of HCHO in the given solution by sodium sulphite method.

Practical-1: 40 Marks, Practical-2: 40 Marks, Note Book: 10 Marks, Viva: 10 Marks.

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

Full Marks: 100

Pass Marks: 50

Time : 06 Hrs

Two questions are to be set.

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, CH₃COOH and CuSO₄ 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 E⁰ 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 CuSO₄ and NH₃.

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.

Practical-1: 40 Marks, Practical-2: 40 Marks, Note Book: 10 Marks, Viva: 10 Marks.

M.Sc. Semester-IV
Core Course – 9 (CC-9)
Synthetic Organic Chemistry

Full Marks: 70+30
Total Lecture: 70 Hours

Eight questions are to be set out of which five are to be answered.

I Retro-synthesis **10 Hrs**

Retro synthetic analysis : Definition, Synthons approach, Synthetic equivalent, Linear and convergent method in organic synthesis, Disconnection approach : One group disconnection, Retro synthesis of alcohols, Retro Diels-Alder reaction, Retro synthesis of olefins, Retro synthesis of aliphatic ketones.

II Pericyclic Reactions **20 Hrs**

Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene, allyl system, Classification of pericyclic reactions. FMO approach, Woodward-Hoffman correlation diagram method and PMO approach for pericyclic reaction under thermal and photochemical conditions.

Electrocyclic reactions: Conrotatory and disrotatory motion, $4n$ and $(4n+2)$ systems, Cycloaddition reaction: $[2+2]$ and $[4+2]$ cycloaddition reaction, Cycloaddition of ketones, Secondary effects in $[4+2]$ cycloaddition. Stereochemical effects on rate of cycloaddition reaction, Diels-Alder reaction, 1,3-dipolar cycloaddition, Chelotropic reaction, The Nazarov reaction.

Sigmatropic rearrangement: Suprafacial and antarafacial shift involving H and carbon-moieties, Peripatetic cyclopropane bridge, Retention and inversion of configuration, $[3,3]$ -, $[1,5]$ -, $[2,3]$ -, $[4,5]$ -, $[5,5]$ -, and $[9,9]$ -Sigmatropic rearrangements, Claisen rearrangements (including Aza-Claisen, Ireland-Claisen), Cope rearrangements (including Oxy-Cope, Aza-Cope), Sommelet-Hauser rearrangements, Group transfer reaction, Ene reaction, Mislow - Evans rearrangement, Walk rearrangement.

III Photochemistry **10 Hrs**

Thermal versus photochemical reactions, Electronic excitations: $n-\pi^*$ and $\pi-\pi^*$ transitions. Singlet and Triplet energy states: Comparison of energies, Lifetimes and Reactivity. Jablonski diagram, Allowed and forbidden transitions: Fluorescence, Phosphorescence, Internal conversion and Intersystem crossing.

Photochemical reactions of saturated ketones : Norrish Type I and Norrish Type II reaction, Photoreduction of ketone, Photoaddition reactions, Paterno-Buchi reaction. Photochemistry of simple olefins : Cis-trans isomerization, Di- π methane rearrangement. Photooxidation : Formation of peroxy compounds, oxidative couplings : Barton reaction. Photo rearrangements : Photo-Fries rearrangement and Photo rearrangement of 2,5-Cyclohexadienones.

IV Reagents in Oxidation Reactions

15 Hrs

DDQ, Oxidation with SeO_2 , Epoxidation of olefins, Sharpless asymmetric epoxidation, Robinson annulations, Dihydroxylation of olefins using KMnO_4 and OsO_4 , Woodward and Prevost dihydroxylation, Oxidative cleavage of olefins, Ozonolysis, (i) Oxidation of alcohols: Chromium reagents, Pyridinium chlorochromate (PCC), Collins and Jones reagent, DCC, Oxidation with MnO_2 , Oppenauer oxidation. (i) Oxidation of aldehydes and ketones: Baeyer-Villiger oxidation, $\text{Pb}(\text{OAc})_4$, Dess-Martin periodinane. (With stereochemistry of oxidation).

V Reagents in Reduction Reactions

15 Hrs

Catalytic hydrogenation: Raney Ni-catalyst, Adam catalyst, Lindlar catalyst, Wilkinson catalyst. (ii) Reduction by dissolving metals: Birch reduction, Hydrogenolysis (iii) Reduction by hydride transfer reagents: MPV reduction, Reduction with LiAlH_4 and NaBH_4 , Diisobutylaluminium hydride (DIBAL-H), Reduction with boranes and derivatives, Reduction with Bu_3SnH , Reduction of carbonyl group to methylene, Reduction with trialkylsilanes. (With stereochemistry of reduction).

Reference Books

1. Jerry March, Advanced Organic Chemistry -Reactions, Mechanisms and Structure , Fourth Edition, John Wiley & Sons (1992)
2. P.S. Kalsi, Organic Reactions and Mechanisms , Second Edition, New Age International Publishers, 2002.
3. P.S. Kalsi, Stereochemistry – Conformation and Mechanism , 6 th Edition, Wiley Eastern Limited, 2005.
4. I.L. Finar, Organic Chemistry , Volume II, Fifth Edition, First Indian reprint, Pearson Education Asia Pte. Ltd., (2000)
5. S.M. Mukherji and S. P. Singh, Reaction Mechanism in Organic Chemistry , 1 st Edition, Macmillan, 1976.
6. R.T. Morrison and R.N. Boyd, Organic Chemistry , Prentice-Hall, 1992.
7. R.O.C. Norman, Principles of Organic Synthesis , Second Edition, Chapman and Hall, 1978.
8. Fundamentals of Photochemistry, K.K. Rohatgi Mukherjee, Wiley Eastern Limited
9. Photochemistry, Carol E Wayne and Richard P Wayne, Oxford University Press(1996)
10. Organic Photochemistry, J. M. Cozen and B. Halton, Cambridge University Press (1st Edition) 1974
11. Molecular Reactions and Photochemistry, C H Deputy and D S Chapman, Prentice Hall India, New Delhi (1st Edition) , 1972.

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

Full Marks: 70+30
Total Lecture: 70 Hours

Eight questions are to be set out of which five are to be answered.

I Metal Clusters, Metal-metal bonding and Metal π -Complexes 20 Hrs

Higher boranes, carboranes, metalloboranes, metallocarboranes and Halide clusters. Polyhedral model of metal clusters, effect of electronic configuration and coordination number. Structures of metal carbonyl clusters of three atoms $M_3(CO)_12$ ($M=Fe, Ru \& Os$), Four metal atoms tetrahedra $M_4(CO)_12$ [$M= Co, Rh \& Ir$] and octahedron of type $M_6(CO)_16$ [$M = Co \& Rh$], and halide derivatives of Rhenium (III) triangles, metal carbonyls involving bridged-terminal exchange and scrambling of CO group. Electron counting in carbonyl clusters, Wades-Mingos and Lauher rules. Vibrational spectra of metal carbonyls for bonding and structure elucidation, Important reactions of metal carbonyls. Preparation, Bonding, Structure and Important reactions of transition metal Nitrosyl, Dinitrogen and Dioxygen complexes. Tertiary phosphine as ligand.

II Metal-Ligand Bonding and Complex metal hydrides 10 Hrs

Limitation of crystal field theory, molecular orbital theory, octahedral, tetrahedral and square planar complexes, p-bonding and molecular orbital theory. Complex metal hydrides, Dissolving metal reductions (including Birch, Benkeser), Diimide reduction, Organoboranes as reducing agents. McMurry reaction. Pummer, Willgerdot, Corey-Bakshi-Shibata and Tishchenko reactions.

III Metallo enzymes 10 Hrs

Structure and reactivity, Apoenzymes, Haloenzyme & Coenzyme. The principle involved and role of various metals in (i) Zn-enzymes: Carboxypeptidase, Carbonicanhydrase and alcoholdehydrogenase. (ii) Fe-enzyme: Catalase Peroxidase & Cytochrome P-450, (iii) Cu-enzyme: Superoxide dismutase (iv) Mo-enzyme: Oxatransferase enzymes, Nitrate reductase and Xanthine oxidase, Structure of vitamin B12, Co-enzyme Vit. B12, Coenzyme: B12r, B12s, biochemical functions of cobalamins, Co-C bond cleavage, Mutase activity of Co- enzyme B-12, Alkylolation reactions of Methyl Cobalamin. Synthetic model of enzyme action, stability and ageing of enzyme.

IV Electron Transfer in Biology 10 Hrs

Electron transfer in Biology: Structure and functions of metalloproteins in electron transfer proteins, Cytochromes, Ferridoxines: 2Fe-2S, Rieske centers, High potential iron proteins; 4Fe-4S, 3Fe-4S, 8Fe-8S, Non-heme iron proteins; Rubredoxins, Synthetic models. Mitochondrial flow of electrons from NADH to oxygen, cytochrome C, Cytochrome C oxidase. Biological Nitrogen fixation (in vitro and in vivo)

- V Chemistry of Main Group Elements** **10 Hrs**
Chemistry of main group elements - Structure and bonding in boranes, carboranes, metallocarboranes, Wades rules, borazines, phosphazenes, S,N-compounds. Silicates-Classification, structures, isomorphous replacement, pyroxenes, layered and vitreous silicates, zeolites and molecular sieves.
- VI Isopoly and Heteropoly acids** **05 Hrs**
Isopoly and heteropoly acids of W, Mo and V, preparations, properties, structure and applications. Stereoisomerism - Chirality, optical activity.
- VII Nitrogenase** **05 Hrs**
Biological nitrogen fixation, molybdenum nitrogenase, spectroscopic and other evidence, other nitrogenases model systems.

Reference Books

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. Comprehensive Coordination Chemistry eds., Q. Wilkinson, R.D. Gillars and J.A. McCleverty, Pergamon.
5. Biochemistry: The Chemical Reactions of Living Cells, D. E. MeUler, Academic Press.
6. Principles of Bioinorganic Chemistry, S.J. Lippard and J.M. Berg, University Science Books.
7. Bioinorganic Chemistry, I. Bertini, H.B. Gray, S.J. Lippard and J.S. Valentine, University Science Books.
8. Bioorganic Chemistry: A Chemical Approach to Enzyme Action, Hermann Dugas and C. Penny, Springer-Verlag.

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

Full Marks: 70+30
Total Lecture: 70 Hours

Eight questions are to be set out of which five are to be answered.

I Conformational Analysis 10 Hrs

Conformational analysis of simple cyclic (chair and boat cyclohexanes) and acyclic (n-butane) systems, conformation of simple 1,2 disubstituted derivatives - ethylene chlorohydrin and ethylene glycol, Conformational analysis and stereochemical features of disubstituted cyclohexanes (1,2- 1,3- 1,4- dialkylcyclohexanes), conformation and stereochemistry of cis- and trans-decalins, effects of conformation on reactivity in acyclic and cyclohexanes.

II Terpenoids and Carotenoids 10 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 and β -carotene.

III Structure Determination and Synthesis of Vit. A, B₂, B₆, Vit. C and Vit. D. 10 Hrs

IV Six-Membered Heterocycles with Two or More Hetero-atoms 10 Hrs

Synthesis and reactions of Pyridazine, Pyrimidine and Pyrazine : Reactions with electrophilic reagents, oxidising agents, nucleophilic reagents, bases, C-metallated diazines, reducing reagents, electrocyclic and photochemical reactions, preparation of N-oxides.

V Six-Membered Heterocycles with one Heteroatom 10 Hrs

Synthesis and reactions of pyrytium salts and pyrones and their comparison with pyridinium & thiopyrylium salts. Synthesis and reactions of benzopyrylium salts.

VI Alkaloids 10 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, Morphine and Narcotine.

VII Steroids 10 Hrs

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

Reference Books

1. The Chemistry of Heterocycles, T. Eicher and S. Hauptmann, Thieme.
2. Heterocyclic Chemistry, J. A. Joule, K. Mills and G.F. Smith, Chapman and Hall.
3. Comprehensive Heterocyclic Chemistry, A. R. Kalriliky and C. W. Rees, eds. Pergamon Press.
4. Natural Products: Chemistry and Biological Significance, J. Mann, R. S. Davidson, J. B. Hobbs, D.V, Banthiropo and J. B. Harbome, Longman,Essex.
5. Organic Chemistry, Vol 2, I. L. Finar, ELB S.
6. Mechanism and Theory in Organic Chemistry, T. H. Lowry and K. C. Richardson, Harper and Row.

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

Full Marks: 70+30
Total Lecture : 70 Hours

Eight questions are to be set out of which five are to be answered.

I Electrochemistry 15 Hrs

Electrochemistry of solution, Debye-Huckel theory of strong electrolytes, Debye-Huckel-Onsager treatment and its extension, ion solvent interactions. Thermodynamics of electrified interface equations. Derivation of electro-capillarity, Lippmann equation (surface excess), methods of determination. Structure of electrified interface. Guoy-Chapman, Stern, Graham-Devnathan-Mottwatts, Tobin, Bockris, Devnathan models. Overpotentials, exchange current density, derivation of Butler-Volmer equation, Tafel plot. Quantum aspects of charge transfer at electrodes-solution interfaces, quantization of charge transtunneling.

II Electrode Deposition 10 Hrs

Electrocatalysis - Electrocatalytic rate, Electrocatalysis in redox system. Total deposition current density, Time variation of the overpotential and rate determining step in electrode deposition. Total overpotential for electrode deposition in steady state. Hydrogen overvoltage, rate determining step of the hydrogen evolution reaction, Determination of reaction order with respect to H^+ ion in solution.

III Corrosion Process 15 Hrs

Introduction, dry and wet corrosion, theories and mechanisms of wet (electrochemical) corrosion, thermodynamic aspects of corrosion, kinetic aspects- determination of rates of corrosion by linear polarization, Tafel extrapolation and impedance techniques. Factors influencing the rate of corrosion-metal and environmental. Methods of corrosion prevention: Cathodic protection, anodic protection, use of corrosion inhibitors, use of organic coatings.

Passivity: Definition, corrent potential diagram, characteristics of passivity, theory and mechanism of passivation, flade potential, trans passivity. Use of ellipsometric technique in the study of passivating films.

IV Electrode Kinetics 15 Hrs

Faradic and non-Faradic current, Rate law, Current density, Factors affecting electrode reaction, Types of overvoltage, Polarisation, Polarisation curves, Electric potential, derivation of Nernst equation (i) On thermodynamic consideration and (ii) By kinetic approach, Nernst diffusion layer treatment, exchange current density, Stoichiometric number, Concept of rate determining step, Energy barriers for multistep reactions, Studies on electrode kinetics-polarographic analysis, Rotating disc convection method.

V Catalysis and Oscillation

15 Hrs

Kinetics of catalytic reactions, Theory of acid-base catalysis, Vant Hoff and Arrhenius complexes, Protogenic and protophilic mechanism, Effect of salt on acid-base catalysis, autocatalysis, 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 reaction, Lotka-Volterra model, B-Z reaction. The Brussel oscillator, bistability, Chemical chaos.

Reference Books

1. Physical Chemistry, Waller J. Moore
2. Physical Chemistry, P.W. Atkins
3. Thermodynamics for Chemists by S. Glasstone, East-West Press, New Delhi
4. Thermodynamics by Rajaraman and Kuriacose, East-West Press
5. Statistical Thermodynamics, M. C. Gupta (Wiley Eastern Ltd.)
6. Elementary Statistical Thermodynamics, N. D. Smith, Plenum Press, NY
7. Elements of Classical and Statistical Thermodynamics, L. K. Nash, Addison-Wiley
8. Modern Electrochemistry Vol-1 and 2, J. O. M. Bockris and A. K. N. Raddy, Plenum New York
9. An Introduction to Electrochemistry, Samuel Glasstone East-West edition New Delhi
10. Text Book of Physical Chemistry, Samuel Glasstone, 2nd edition, Mac Millan India Ltd.
11. Electrochemistry: Principles and Applications, Edmund, C. Potter, Cleaver, Hume press London
12. Principles and Applications of Electrochemistry, D. R. Crow, 3rd edition, Chapmanhall London

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

Full Marks: 100

Pass Marks: 50

Time : 12 Hrs

Two questions are to be set.

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 simple inorganic complexes, their purification, Molecular Weight determination and elucidation of the structures by available physical methods.

- (a) Preparation of Cobalt (III) complexes
 - (i) $[\text{Co}(\text{NH}_3)_5\text{Cl}]\text{Cl}_2$
 - (ii) $[\text{Co}(\text{NH}_3)_5\text{NO}_2]\text{Cl}_2$
 - (iii) $[\text{Co}(\text{NH}_3)_5\text{ONC}]\text{Cl}_2$
- (b) Preparation and characterisation of Cr(III) complexes
 - (i) $[\text{Cr}(\text{H}_2\text{O})_6]\text{NO}_2 \cdot \text{H}_2\text{O}$
 - (ii) $[\text{Cr}(\text{H}_2\text{O})_4\text{Cl}_2]\text{Cl} \cdot \text{H}_2\text{O}$
 - (iii) $\text{Cr}(\text{acac})_3$
- (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 spectroscopy)
- (e) Preparation of mercury tetrathiocyanato cobaltate : $\text{Hg}[\text{Co}(\text{CNS})_4]$

IV Determination of

- (a) Manganese/Chromium/Vanadium in steel sample by spectrophotometric method
- (b) Ni/Mo/W/V/U by extractive spectrophotometric method.

V Flame Photometric Determinations

- (a) Sodium and Potassium when present together
- (b) Li/Ca/Ba/Sr Naphelometric determinations
- (c) Sulphate
- (d) Phosphate
- (e) Silver

Practical-1: 40 Marks, Practical-2: 40 Marks, Note Book: 10 Marks, Viva: 10 Marks.

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

Full Marks: 100

Pass Marks: 50

Time: 12 Hrs

Two questions are to be set.

I Organic Synthesis and Extraction of Organic Compounds from Natural Sources:

The students are expected to carry out 6 to 8 organic preparations/isolation (usually involving not more than two steps). 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.

Some of the illustrative experiments are listed below:

Extraction:

1. Extraction of Caffeine from Tea Leaves.
2. Isolation of Casein from Milk.
3. Isolation of Lactose from Milk.
4. Isolation of Nicotine dipicrate from Tobacco.
5. Isolation of Cinchonine from Cinchona bark
6. Isolation of β -Carotene from Carrots
7. Isolation of Oleic acid from Olive oil
8. Isolation of Eugenol from Cloves

Preparation:

1. Synthesis of 3-Nitrobenzoic acid from Benzoic acid.
2. Preparation of Indigo from Anthranilic acid.
3. Cannizzaro reaction of 4-Chlorobenzaldehyde.
4. Synthesis of Benzanilide from Benzene.

Make a comparative study of the IR and PMR spectra of starting materials as well as products, if possible.

II 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 $\text{Na}_2\text{CO}_3\text{-KNO}_3$ 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
7. To determine the percentage or number of hydroxyl groups in the given sample by the acetylation method.

Practical-1: 40 Marks, Practical-2: 40 Marks, Note Book: 10 Marks, Viva: 10 Marks.

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

Full Marks: 100

Pass Marks: 50

Time: 12 Hrs

Two questions are to be set.

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 $Na_2SO_4 \cdot 10 H_2O$.

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

Practical-1: 40 Marks, Practical-2: 40 Marks, Note Book: 10 Marks, Viva: 10 Marks.

M.Sc. Semester-IV

PROJECT

Full Marks: 100

Time: 06 Hrs

The paper will consist of

- (a) Field work/Lab work related to the project.
- (b) Preparation of dissertation based on the work undertaken.
- (c) Presentation of project work in the seminar on the assigned topic in the University Department of Chemistry, DSPM University, Ranchi & open viva there on.

NB:- The students will select topic for the project work in consultation with a teacher of the Department.

Topics

Project work related to the following Industrial/Social relevant topics may be given to the students of M.Sc. SEM-IV in Paper-XVI

- (a) Environmental study such as
 - (i) Analysis of water, soil, air etc.
- (b) Industrial goods analysis such as
 - (i) Analysis of Cement
 - (ii) Analysis of minerals/coal available in Jharkhand State
 - (iii) Synthesis of useful commercial products based on raw materials available in Jharkhand state such as Lac, lime-stone etc.
 - (iv) Isolation of constituents of Medicinal plants available Jharkhand State.

Each student has to submit two copies of the dissertation work duly forwarded by the HOD. The forwarded copies will be submitted in the University Department of Chemistry, DSPM University, for evaluation (Seven days before the seminar).