

M.J.P. Rohilkhand University Bareilly

Rules and Regulations regarding M.Sc. Chemistry course starting from session 2022-23

Course/program structure:

- There will be only **one Major Subject** in Post graduate program.
- **Postgraduate** program will run under **C.B.C.S. and semester system**.
- There will be **four theory papers** (each of 4 credit) leading to 16 credits in each semester. Lab exercises would comprise of 6 credits in each semesters. In addition, there will be 6 credits for project/ dissertation in each third and fourth semester.
- In the second semester, there will be one optional paper.
- In the 3rd and 4th semester of post graduate program, students will have to opt for 2 elective papers based on specialization as per his/her choice, available in the institution. These paper will be of 4 credits.

Research project in postgraduate program:

- Student will have to do a research dissertation/ project related to major subject elected by him in 3rd and 4th semester.
- This research project may be interdisciplinary/ multidisciplinary. It may be in the form of Industrial training/ internship/ survey work etc.
- The research project must be completed under supervision of the college faculties. If necessary, the students can take a joint support in supervision from any concern industrial/ corporate/ technical or research institute personnel.
- The research project/ seminar would be of 6 credits each in 3rd and 4th semester.
- **Excursion tour** for PG students of 3rd semester will be organized for visiting various industrial units/ research institutions under the supervision of faculties. Students must submit one page report and presentation about the tour. The tour should be financed by both the students and the institutes.

Credit determination and attendance:

- To obtain postgraduate degree, it will be necessary to obtain minimum 44 credits in

Ist year and 56 credits in IInd year. The division of credits will be as follows:

I year (44 credits)

I semester-

- $4 \times 4 = 16$ credits for core papers
- 6 credits for Lab work
- **Total 22 credits**

II semester-

- $3 \times 4 = 12$ credits for core papers
- 4 credits for 1 optional paper
- 6 credits for Lab work & seminar
- **Total 22 credits**

II year (56 credits)

III semester-

- $2 \times 4 = 8$ credits for core papers
- $2 \times 4 = 8$ credits for elective papers
- 6 credits for Lab work & seminar
- 6 credits for Project
- **Total 28 credits**

IV semester-

- $2 \times 4 = 8$ credits for core papers
- $2 \times 4 = 8$ credits for elective papers
- 6 credits for Lab work & seminar
- 6 credits for Project/ Dissertation
- **Total 28 credits**

➤ **Thus, in total there are $44+56 = 100$ credits.**

- It will be necessary to give exam for credit validation. The credits will be incomplete without examination. The 75 percent attendance will be compulsory for appearing in the examination.

If a student is eligible for giving exam on the basis of attendance, but unable to give exam

due to any reason, then he may participate in the exam in the coming session. There is no need of taking classes again.

The other rules concerned to credits will be according to rules and regulations issued earlier.

Evaluation:

- Every paper in each semester will be prepared for 100 marks.
- All the core/optional/elective subjects will be evaluated externally and internally both.
- Out of 100 max. marks, 30 marks will be awarded for internal evaluation and 70 marks for external evaluation.
- For internal evaluation, a written test of 20 marks will be conducted. 5 marks will be awarded for assignment and remaining 5 marks will be given on the basis of attendance and conduct of student in the class.
- On the basis of research project done in 3rd and 4th semester, the prepared project report/dissertation will be evaluated by external and internal examiners in 100 marks in both the semesters.

Program Outcomes:

The purpose of the syllabus is to

- Solve and understand of major concepts in all disciplines of Chemistry independently and in group as well as draw logical conclusions through Project and Seminar Presentation.
- Employ critical thinking and the scientific knowledge to design, carry out, record and analyze the results of Chemistry experiments.
- Equip students to face the employment challenges and instill confidence to turn into entrepreneur and also step into research career.
- Generate new scientific insights or to the innovation of new applications of chemical research.
- Apply modern methods of analysis to chemical systems in a laboratory setting.
- Enhance students' ability to develop global level research opportunities to pursue Ph.D. program targeted approach of CSIR/UGC – NET examination and specific competitive exams conducted by service commission.

COURSE TABLE FOR M.Sc. CHEMISTRY SYLLABUS

SEMESTER –I			
COURSE CODE	PAPER NUMBER	PAPER NAME	CREDIT/ MAX. MARKS
MCHC-101	PAPER- I	Inorganic Chemistry	4/100 (70 + 30)
MCHC-102	PAPER- II	Organic Chemistry	4/100 (70 + 30)
MCHC-103	PAPER- III	Physical Chemistry	4/100 (70 + 30)
MCHC-104	PAPER- IV	Group Theory	4/100 (70 + 30)
MCHL-105	PAPER- V	Practical & Seminar	6/100 (70 + 30)
			Total =22/500

SEMESTER –II			
COURSE CODE	PAPER NUMBER	PAPER NAME	CREDIT/MAX. MARKS
MCHC-201	PAPER- I	Inorganic Chemistry	4/100 (70 + 30)
MCHC-202	PAPER- II	Organic Chemistry	4/100 (70 + 30)
MCHC-203	PAPER- III	Physical Chemistry	4/100 (70 + 30)
MCHO-204	PAPER- IV	Instrumental Chemistry	4/100 (70 + 30)
MCHO-205	PAPER- V	Environmental Chemistry	4/100 (70 + 30)
MCHL-206	PAPER- VI	Practical & Seminar	6/100 (70 + 30)
			Total =22/500

SEMESTER –III				
COURSE CODE	PAPER NUMBER	PAPER NAME	PAPER TITLE	CREDIT/ MAX. MARKS
MCHC-301	PAPER- I	Spectroscopy	Spectroscopy-1	4/100 (70 + 30)

MCHC-302	PAPER- II	Recent Trends	Recent Trends in Chemistry	4/100 (70 + 30)
MCHE-303	PAPER- III	Inorganic Chemistry	Organotransition Metal Chemistry	4/100 (70 + 30)
MCHE-304	PAPER- IV	Inorganic Chemistry	Analytical & Coordination Chemistry	4/100 (70 + 30)
MCHE-305	PAPER- III	Organic Chemistry	Organic Synthesis-1	4/100 (70 + 30)
MCHE-306	PAPER- IV	Organic chemistry	Heterocyclic Compounds & Photo chemistry	4/100 (70 + 30)
MCHE-307	PAPER- III	Physical Chemistry	Chemistry Material of	4/100 (70 + 30)
MCHE-308	PAPER- IV	Physical Chemistry	Statistical Thermodynamics & chemical kinetics	4/100 (70 + 30)
MCHL-309	PAPER - V	Practical/Seminar		6/100 (70+30)
MCHP-310	PAPER - VI	Dissertation/Project	Research Work	6/100 (70+30)
				Total =28/600

SEMESTER-IV				
COURSE CODE	PAPER NUMBER	PAPER NAME	PAPER TITLE	CREDIT/ MAX. MARKS
MCHC-401	PAPER I	Spectroscopy	Spectroscopy-II	4/100 (70 + 30)
MCHC-402	PAPER II	Green Chemistry	Green Chemistry	4/100 (70 + 30)
MCHE-403	PAPER III	Inorganic Chemistry	Photo Inorganic &supramolecular Chemistry	4/100 (70 + 30)
MCHE-404	PAPER IV	Inorganic Chemistry	Bioinorganic Chemistry	4/100 (70 + 30)
MCHE-405	PAPER III	Organic Chemistry	Organic Synthesis- II	4/100 (70 + 30)

MCHE-406	PAPER IV	Organic Chemistry	Chemistry of Natural Product	4/100 (70 + 30)
MCHE-407	PAPER III	Physical Chemistry	Advanced Quantum Chemistry	4/100 (70 + 30)
MCHE-408	PAPER IV	Physical Chemistry	Polymer Chemistry	4/100 (70 + 30)
MCHL-409	PAPER - V	Practical/Seminar		6/100 (70+30)
MCHP-410	PAPER - VI	Dissertation/ Project	Research Work	6/100 (70+30)
				Total 28/600

Abbreviations:

MCHC : M.Sc. Chemistry Core paper

MCHL :M.Sc. Chemistry
Lab

MCHO : M.Sc. Chemistry Optional paper

MCHP : M.Sc. Chemistry
Research Project

MCHE : M.Sc. Chemistry elective paper

In course code:

Ist letter (M) : Master degree (M.Sc.)

IInd and IIIrd letter (CH) : Subject code (Chemistry)

IV letter (C,O,L,P,E) : Nature of course

(C: Core paper, O: Optional, L: Lab, P: Research Project, E: elective paper)

In Code Number:

101: First Number: Semester

Last number: paper number

Semester 1

Paper-I: MCHC-101

Inorganic Chemistry

60 Hrs

(I) Stereochemistry and Bonding in Main Group Compounds

10 Hrs

VSEPR, Walsh diagrams (tri- and penta- atomic molecules) $d\pi - p\pi$ bonds, bent rule and energetic of hybridization.

(II) Reaction Mechanism of Transition Metal Complexes

26 Hrs

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, agnation reactions, reactions without metal ligand and bond cleavage. Substitution reactions in square planer complexes, the trans effect, mechanism of the substitution reaction. Redox reaction, electron transfer reactions, outer sphere type reaction, inner sphere type reactions.

(III) Metal-Ligand Equilibria in Solution **14 Hrs**

Stepwise and overall formation constants and their interaction, trends in stepwise constants, factors affecting the stability of metal complexes with references to the nature of metal ion and ligand, chelate effect and its thermodynamic origin, determination of binary formation constants by pH- metry a spectrophotometry.

(IV) Metal-ligand Bonding **10 Hrs**

Limitations of CFT, molecular orbital theory, octahedral, tetrahedral and square planner complexes. π -bonding and molecular orbital theory.

Books Suggested

1. Advanced Inorganic Chemistry, F.A. Cotton and Wilkinson, John Wiley.
2. Inorganic chemistry, J.E. Huheey, Harpes & Row.
3. Chemistry of the Elements N.N. Greenwood and A. Earnshaw, Pergamon.
4. Inorganic Electronic Spectroscopy, A.B.P. Lever, Elsevier.
5. Magnetochemistry, R.L.Carlin, Springer Verlag.
6. Comprehensive Coordination Chemistry eds, G. Wilkinson, R.D.Gillers and J.A. McCleverty, Pergamon.

PAPER-II: MCHC-102

Organic Chemistry **60 Hrs**

(I) Nature of Bonding in Organic Molecules **10 Hrs**

Delocalized chemical bonding - conjugation, cross conjugation, resonance, hyperconjugation, bonding in fullerenes tautomerism. Aromaticity in benzenoid and non-benzenoid compounds

alternant and non-alternant hydrocarbons. Huckel's rule, homo-aromaticity, energy level of π - molecular orbitals, annulences, anti-aromaticity, Ψ -aromaticity, homo-aromaticity, PMO approach Bonds weaker than covalent-addition compounds.

(II) Reaction Mechanism: Structure and Reactivity

10 Hrs

Types of mechanism, types of reactions, thermodynamic and kinetic requirements, kinetic and thermodynamic control. Potential energy diagrams, transition states and intermediates, methods of determining mechanism, 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. The Hammett equation and linear free energy relationship, substituent and reaction constants.

(III) Aliphatic Nucleophilic Substitution

12 Hrs

The S_N2 , S_N1 , mixed S_N1 and S_N2 and SET mechanisms. The neighbouring group mechanism, neighbouring group participation by π and σ bonds, anchimeric assistance. Classical and nonclassical carbocations, phenonium ions, norbornyl system, common carbocation rearrangements. Application of NMR spectroscopy in the detection of carbocations. Nucleophilic substitution at an allylic, aliphatic trigonal and a vinylic carbon. Reactivity effects of substrate structure, attacking nucleophile, ambident nucleophile, leaving group and reaction medium, phase transfer catalysis, regioselectivity.

(IV) Aromatic Nucleophilic Substitution

6 Hrs

The S_{NAr} , S_N1 benzyne and $SRN1$ mechanisms. Reactivity- effect of substrate structure, leaving group and attacking nucleophile. The von-Richer, sommelet- Hauser and Smiles rearrangements.

(V) Aliphatic Electrophilic Substitution

6 Hrs

Bimolecular mechanisms- SE_2 and SE_1 mechanism, SE_i . electrophilic substitution accompanied by double bond shifts. Effect of substrates, leaving group and the solvent polarity on the reactivity.

(VI) Aromatic Electrophilic Substitution

6 Hrs

The arenium ion mechanism, orientation and reactivity, energy profile diagrams. The ortho/para ratio, ipso attack, orientation in other ring systems. Diazonium coupling, 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, neighboring 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.

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.O. House, Benjamin.
7. Principles of Organic Synthesis, R.O.C. Norman and J. M. Coxon, Blackie Academic & Professional.
8. Reaction Mechanism in Organic Chemistry, S. M. Mukherji and S. P. Singh, Macmillan.

PAPER-III: MCHC-103

Physical Chemistry

60 Hrs

(I) Introduction to Exact Quantum Mechanical Results

15 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.

(II) Approximate Methods **5 Hrs**

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

(III) Angular Momentum **10 Hrs**

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.

(IV) Electronic Structure of Atoms **15 Hrs**

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.

(V) Molecular Orbital Theory **15 Hrs**

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

Books Suggested

1. Physical Chemistry, P.W. Atkins, ELBS.
2. Introduction to Quantum Chemistry, A.K. Chandra. Tata McGraw Hill.
3. Quantum Chemistry, Ira N. Levine, Perntice Hall.
4. Quantum Chemistry, Donald A Mcquarrie.
5. Principles of Physical Chemistry, Puri, Sharma, Pathania. Vishal Publishing Co.

PAPER-IV: MCHC-104

Group Theory **60 Hrs**

(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 C_n , C_{nv} , C_{nh} ,

D_{nh} 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.

(II) X-ray Diffraction

15 Hrs

Bragg condition, Miller indices, Laue method, Bragg method, Debye-Scherrer method of X-ray structural analysis of crystals, index

reflections, identifications of unit cells from systematic absence in diffraction pattern, Structure of simple lattices and x-ray intensities, structure factor its relation to intensity and electron density, phase problem, Description of the procedure for an X-ray structure analysis, absolute configuration of molecules, Ramachandran diagram.

(III) Electron Diffraction

10 Hrs

Scattering intensity vs. scattering angle, wierl equation measurement technique, elucidation of structure of simple gas phase molecules. Low energy electron diffraction and structure of surfaces.

(IV) Neutron Diffraction

10 Hrs

Scattering of neutrons by solids and liquids, magnetic scattering, measurements techniques. Elucidation of structure of magnetically ordered unit cell.

Books suggested

1. Modern Spectroscopy, J.M.Hollas, John Wiley.
2. Physical Methods in Chemistry, R.S. Drago, Saunders College.
3. Chemical Applications of Group Theory, F.A.Cotton.
4. Basic principles of spectroscopy, R.Chang. McGraw Hill.
5. DM Bishop, "Group Theory and Chemistry" Dover Publication.

PAPER – V: MCHL-105

Ist SEM. PRACTICAL

Time Duration: 12 Hours in two days

MAX MARKS: 100

Inorganic chemistry exercise

1 - Qualitative analysis of inorganic mixture containing 7 radicals

2 - Separation of cations by following chromatography techniques

A - Paper chromatography

B - Column chromatography

C - Ion exchange chromatography

D - TLC (Thin Layer Chromatography)

Organic chemistry exercise

1 - Separation purification and identification of Organic mixture for two components mixture

2- Organic synthesis:

A - Oxidation (as sugar to oxalic)

B - Nitration (as nitro benzene to meta-dinitro-benzene)

C - Acetylation (as salicylic acid to aspirin)

D - Sandmeyer reaction (as p-Toluedine to p- Chloro Toluedine)

E - Esterification Amyl Acetate

Physical chemistry exercise

1 - Error Analysis and statistical data analysis.

2 - Determination of percentage composition of a given mixture of two liquid by surface tension measurement.

3 - Determine the heat of solution of $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$.

4 - Determine the rate constant by hydrolysis of ester volumetrically.

Marks Distribution for Lab. Course for M.Sc. I Sem.

A - Inorganic Chemistry exercise - 15 Marks

B - Organic Chemistry exercise - 15 Marks

C - Physical Chemistry exercise - 15 Marks

D - Attendance + Record + Viva - 15 Marks

E - Seminar - 10 Marks

External Total - 70 Marks

Internal Total - 30 Marks

Semester 2

PAPER-I: MCHC-201

Inorganic Chemistry **60 Hrs**

(I) Electronic Spectra and Magnetic Properties of Transition Metal Complexes 20 Hrs

Spectroscopic ground states, Orgel and Tanabe- Sugano diagrams for transition metal complexes (d^1 - d^9 states), charge transfer spectra, anomalous magnetic moments, magnetic exchange coupling and spin crossover.

(II) Metal π - Complexes **18 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 Clusters **12 Hrs**

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

(IV) Inorganic Polymers **10 Hrs**

Silicates, Silicones, Isopoly and Heteropoly acids and Salts

Books Suggested

1. Advanced Inorganic Chemistry, F.A. Cotton and Wilkinson, John Wiley.
2. Inorganic chemistry, J.E. Huhey, Harpes & Row.
3. Chemistry of the Elements N.N. Greenwood and A. Earnshaw, Pergamon.
4. Inorganic Electronic Spectroscopy, A.B.P. Lever, Elsevier.
5. Magnetochemistry, R.L.Carlin, Springer Verlag.
6. Comprehensive Coordination Chemistry eds, G. Wilkinson, R.D.Gillers and J.A. McCleverty, Pergamon.

PAPER-II: MCHC-202

Organic Chemistry **60Hrs**

(a) Stereochemistry **20 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, allens and spiranes), chirality due to helical shape. Stereochemistry of the compounds containing nitrogen, sulphur and phosphorus.

(b) Addition to Carbon- Carbon Multiple Bonds

5 Hrs

Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, regio- and chemoselectivity, orientation and reactivity. Addition to cyclopropane ring. Hydrogenation of double and triple bonds, hydrogenation of aromatic rings. Hydroboration, Mercuration and Demercuration, Michael reaction, epoxidation.

(c) Addition to Carbon- Hetero Multiple Bonds

11 Hrs

Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters and nitriles. Addition of Grignard reagents, organozinc and organolithium reagents to carbonyl and unsaturated carbonyl compounds. Wittig reaction. Mechanism of condensation reactions involving enolates- Aldol, Knoevenagel, Claisen, Perkin and Stobbe, Benzoin, mannich reaction. Hydrolysis of esters and amides, ammonolysis of esters.

(d) Elimination Reactions

4 Hrs

The E₂, E₁, E_{1cB} mechanisms. Orientation of the double bond. Reactivity- effects of substrate structures, attacking base, the leaving group and the medium. Mechanism and orientation in pyrolytic elimination (E_i).

(e) Pericyclic Reactions

20 Hrs

Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3- butadiene, 1,3,5- hexatriene and allyl system. Classification of pericyclic reactions. Woodward- Hoffmann correlation diagrams. FMO and PMO approach. Electrocyclic reactions- conrotatory and disrotatory motions, 4n, 4n+2 and allyl systems. Cycloadditions- antarafacial and suprafacial additions, 4n and 4n+2 systems, 2+2 addition of ketenes, 1,3 dipolar cycloadditions and cheletropic reactions. Sigmatropic rearrangements- suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon

moieties, 3,3- and 5,5 – sigmatropic rearrangements, claisen, cope and aza-cope rearrangements. Fluxional tautomerism, Ene 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.O. House, Benjamin.
7. Principles of Organic Synthesis, R.O.C Norman and J.M. Coxon, Blackie Academic & Professional.
8. Pericyclic Reactions, S.M. Mukherji, Mecomilan, 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.

PAPER-III: MCHC-203

Physical Chemistry

60 Hrs

(I) Classical Thermodynamics

20Hrs

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 coefficient, Debye-Huckel theory for activity coefficient of electrolytic solutions; determination of activity and activity coefficients; ionic strength. Application of phase rule to three component systems; second order phase transitions.

(II) Electrochemistry

20 Hrs

Electrochemistry of solutions, Debye-Huckel- Onsager treatment and its extension, ion solvent

interactions. Debye-Huckel-Jerum mode. Thermodynamics of electrified interface equations. Derivation of electrocapillarity, Lippmann equations (surface excess), methods of determination. Structure of electrified interfaces. Guoy- Chapman, Stern, Helmholtz models. Over potentials, exchange current density, derivation of Butler- Volmer equation, Tafel plot. Quantum aspects of charge transfer at electrode solution interfaces, quantization of charge transfer, tunneling. Semiconductor interfaces- theory of double layer at semiconductor, electrolyte solution interfaces, structure of double layer interfaces. Effect of light at semiconductor solution interface. Polarography theory, Ilkovic equation; half wave potential and its significance.

(III) Surface chemistry

20 Hrs

A. Adsorption

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

B. Macromolecules

Polymer- definition, types of polymers, electrically conducting, fire resistant, liquid crystal polymers, kinetics of polymerization, mechanism of polymerization. Molecular mass, number and mass average molecular mass, molecular mass determination (osmometry, viscometry, diffusion and light scattering methods), sedimentation, chain configuration of macromolecules, calculation of average dimensions of various chain structures.

Books Suggested

1. Physical Chemistry, P.W. Atkins, ELBS.
2. Chemical Kinetics, K.L. Laidier, Mcgraw- Hill.
3. Kinetics and Mechanism of Chemical Transformation, J. Rajaraman and J. Kuriacose, McMillian.
4. Micelles, Theoretical and Applied Aspects, V. Morol, Plenum.
5. Modern Electrochemistry Vol. I and II. J.O.M Bockris and A.K.N. Reddy, Plenum.
6. Principles of Physical Chemistry, Puri, Sharma, Pathania. Vishal Publishing Co.

PAPER-IV: MCHO-204

Instrumental Chemistry

60 Hrs

1. Electroanalytical Techniques:

25 Hrs

(a) **Conductometric:** Discussion of the nature of the curves of acid-base (including mixtures of acids), precipitation and complexometric titrations.

(b) **Potentiometric:** different types of electrodes, discussion of nature of the curves for oxidation-reduction and acid-base titrations, comparison with the conductometric method.

(c) **Voltammetry:** Cyclic voltammetry

(d) **Polarography:** Dropping mercury electrodes and its advantages, polarographically active species, concept of residual, diffusion and limiting current of half-wave potential, Ilkovic equation and factors affecting diffusion current.

2. Thermo-analytical Methods:

20 Hrs

(a) Thermo-gravimetry:

apparatus, factors affecting TGA, interpretation of TG curves of $\text{CaC}_2\text{O}_4 \cdot \text{H}_2\text{O}$ and $\text{MgC}_2\text{O}_4 \cdot 2\text{H}_2\text{O}$

(b) Differential Thermal Analysis:

Apparatus, factors affecting DTA curves with special reference to heating rate, Particle size and packing, measurement of heat of transition, heat of reaction and heat of dehydration of salts of metal hydrates.

3. Radiochemical methods:

10 Hrs

(a) Isotope Method

(b) Inverse Isotopic Dilution

(c) Neutron activation technique.

4. Chromatographic Method:

5 Hrs

(a) Gas Chromatography: GLC and GC

(c) HPLC

Books Recommended:

1. Fundamentals of analytical chemistry, D.A. Skoog, D.M. West and F.J. Holler

2. Quantitative inorganic analysis, A.I. Vogel

3. Instrumental Methods of Chemical Analysis, B.K. Sharma
4. Instrumental Methods of Chemical Analysis, H. Kaur
5. Analytical Chemistry, Gary D. Christian

PAPER-V: MCHO-205

Environmental Chemistry

60 HRS

UNIT-I: Sources of Energy

10HRS

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. Bio distribution of elements. Fossil fuels- Nuclear fission and fusion- Solar energy-use of solar energy in space heating and water heating- production of electricity using solar energy. Hydropower- wind power- Biomass energy- production of ethanol from biomass- production of methane from biomass- photosynthesis- photo electro chemistry- Geothermal energy.

UNIT-II: Environmental Pollution and Control

20 HRS

WATER: Chemical Composition of Water bodies, Aquatic Pollution :- Inorganic, Organic, Pesticide, Agricultural, Industrial and Sewage, detergents, oil spills and oil pollutants, Water quality parameters-dissolved oxygen, biochemical oxygen demands, solids metals, content of chloride, Sulphate, phosphate, nitrate and micro-organisms water quality stand Analytical methods for measuring BOD, DO, COD, F, Oil, Metals (As, Cd, Cr, Hg, Pb, Se etc) residual chloride and chlorine demand, Purification and treatment of water.

AIR: Classification and properties of air pollutants-emission sources-major emissions from global sources importance of anthropogenic sources-behavior and fate of air pollutants photochemical smog and its effects on health-vegetation-material damage in India. Global warning- Ozone depletion – Green house effect, “CFC”s- Acid rain.

UNIT-III: Soil Pollution

5HRS

Soil: Composition of soil- lithosphere- inorganic and organic contaminants in the soil-

Biodegradation- Non degradable waste and its effect on the environment- Bioremediation –of surface soils. Pollution- fertilizers, pesticides.

UNIT-IV: Noise Pollution & industrial Pollution

10 HRS

Noise pollution: sources-measurement of noise and indices-effect of meteorological parameters on noise propagation-noise exposure levels and standards –measurement of noise-impact of noise on human health.

Industrial Pollution: 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. Environmental Toxicology. Chemical solution to environmental problems, biodegradability, principles of decomposition, better industrial processes.

UNIT IV: Environmental Management and Important Environmental Laws 15 HRS

Environmental Management: Introduction-objectives-components-environmental impact assessment (EIA)-historical background-elements of EIA process-participants in EIA processes contents of EIS-design of EIA. Important Environmental Laws: the world life act-the forest conservation act-the water and control pollution act-air prevention& control act—the environment act-environmental quality management standard-ISO 14000 series.

Recommended Books:

1. Manahan, Stanley E. Fundamentals of Environmental Chemistry Boca Raton: CRC Press LLC, 2001
2. Sonja Krause, Herbert M. Clark, James P. Ferris, Robert L. Strong Chemistry of the Environment, Elsevier Science & Technology Books 2002
3. Eugene R. Weiner Applications of Environmental Chemistry 2000 CRC Press, LLC
4. By Clair, N. Sawyer, Perry L. Mc Carty, Gene F. Parking Chemistry for environmental engineering and Science (5th edition) McGraw Hill Professional.

PAPER-VI: MCHL-206

IInd SEM. PRACTICAL

Time Duration: 12 Hours in two days

Max Marks: 100

Inorganic chemistry exercise

1 – Preparation of coordination compounds and their characterization by U.V. & I.R. spectra.

A – Prussian blue, turn bulls blue.

B – $[\text{Cu}(\text{NH}_3)_4]\text{SO}_4 \cdot \text{H}_2\text{O}$

C- $\text{K}_3[\text{Fe}(\text{C}_2\text{O}_4)_3] \cdot 3\text{H}_2\text{O}$

D – $[\text{Ni}(\text{NH}_3)_6]\text{Cl}_2$

E – Cis – $[\text{Cr}(\text{C}_2\text{O}_4)_2(\text{H}_2\text{O})_2]$

F - $\text{Ni}(\text{dmg})_2$

G- Sodium amide

H- Ferrocene

2- Separation and determination of following two constituents present together by using gravimetric and volumetric method.

A – Cu^{2+} and Ni^{2+}

B – Cu^{2+} and Zn^{2+}

C – Ni^{2+} and Zn^{2+}

Organic chemistry experiment

1 – Estimation of amines / Phenol using bromate – bromid solutions or acylation method

2- Extraction of Organic compound from natural sources.

A – Isolation of caffeine from Tea leaf

B – Isolation of caseine and lactose from milk

C – Isolation of nicotine from tobacco

D – Isolation of piperine from cinchona bark.

E - Isolation of Limonene from citrus fruits.

Physical chemistry exercise

- 1 – Determine Enthalpy of Neutralization of Strong acid and strong base.
- 2 – Determine the velocity of hydrolysis of ethyl acetate by sodium hydroxide (Saponification of an ester)
- 3 – Obtain the calibration curve for a given compound by colorimeter and hence verify
a- Beer-Lamberts law b- Percentage composition of the given compound.
- 4 – To Determine Partition coefficient of Benzoic acid between water and Benzene.

Marks Distribution for Lab. Course for M.Sc. I Sem.

A - Inorganic Chemistry exercise – 15 Marks

B - Organic Chemistry exercise – 15 Marks

C - Physical Chemistry exercise – 15 Marks

D - Attendance + Record + Viva – 15 Marks

E - Seminar – 10 Marks

External Total – 70 Marks

Internal Total – 30 Marks

Semester 3

PAPER-I: MCHC-301

Spectroscopy -1

60 Hrs

(I) UV-Visible Spectroscopy

15 Hrs

Different type of electronic transitions, Lambert's Beer's law, Chromophores, Auxochromes, Solvent effect, Red shift and blue shift, Woodward's rule for conjugated cyclic and acyclic dienes and α , β – unsaturated carbonyl compounds, Absorption in aromatic compounds (substituted benzene, naphthalene and anthracene), Problems related UV-Visible Spectroscopy

(II) Infrared Spectroscopy

15 Hrs

Review of linear harmonic oscillator, Vibrational energies of diatomic molecules, Zero point energy, Force constant and bond strength, Anharmonicity, Morse potential energy diagram, Vibration rotation spectroscopy, P, Q, R branches, Break down of Born-Oppenheimer

approximation, Selection rules, Overtones, Hot Bands, Absorption by common functional groups, Brief description of IR and F.T.I.R. instruments, Problems related I.R. Spectroscopy

(III) Raman Spectroscopy

15 Hrs

Theories of Raman Effect, Conditions of Raman active Vibrations, Selection rules, Polarized and Depolarized Raman lines Study of : (Simple molecules such as SO₂, CO₂, N₂O and C₂H₂; (b) Hydrogen Bonding and (c) Metal ions in solution, Mutual exclusion principle, Problems related with Raman Spectra and its interpretation

(IV) Microwave spectroscopy

15 Hrs

Rotational Spectroscopy, Rotational spectra of diatomic molecules based on rigid rotator approximation, Determination of bond lengths and/or atomic masses from microwave data, Effect of isotopic substitution, Non-rigid rotator, Classification of polyatomic molecules, Energy levels and spectra of symmetric top molecules and asymmetric top molecules and applications.

Books suggested

1. Modern Spectroscopy, J. M. Hollas, John Wiley.
2. Applied Electron Spectroscopy for Chemical Analysis Ed. H. Windalwl and F. L. Ho. Wiley Interscience.
3. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R. V. Parish, Ellis Harwood.
4. Physical Methods in Chemistry, R.S. Drago, Saunders College.
6. Introduction to Molecular Spectroscopy, G.M. Barrow. McGraw Hill.
7. Basic principles of spectroscopy, R. Chang. McGraw Hill.
8. Theory and Applications of UV Spectroscopy, H.H. Jaffe and M. Orchin, IBH-Oxford.

PAPER-II: MCHC-302

Recent trends in Chemistry

60 Hrs

1. Nanoscience:

15 Hrs

Introduction of nanotechnology, Nanostructures : Carbon Nanotubes (CNT), Graphenes, Fullerenes, metallic nanoparticle, Nano Peapods, Quantum Dots and Semiconductor Polymer-

based dendrimers, sphere and fiber, Nanomaterial for energy storage application.

2. Sonochemistry

15 Hrs

Sound properties, Bubble formation, Ultrasound, principles of Sonochemistry and acoustic cavitation, Interfaces and Bubbles, Sonoluminescence, Bubble Temperature Estimation Homogeneous (liquid- phase) and heterogeneous (solid surface-liquid, particle liquid and liquid-liquid) reactions.

3. Metals in Medicine

10 Hrs

Metal deficiency diseases, toxic effects of metals, metals used for diagnosis and chemotherapy with particular reference to anticancer drugs.

4. Drug Design

20 Hrs

Development of new drugs, clinical trial I, II, III & IV, ADME principle, introduction to computer aided drug design, solubility & permeability, drug likeness, pharmacophore, Lipophilicity, Structure activity relationship (SAR), Factors affecting bioactivity, isosterism, bioisosterism, spatial considerations, Theories of drug activity, Occupancy theory, rate theory, induced fit theory.

PAPER-III: MCHE-303

Inorganic Chemistry (Organotransition Metal Chemistry) 60 Hrs

(I) Alkyls and Aryls of Transition Metals 5 Hrs

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

(II) Compounds of Transition Metal-Carbon Multiple Bonds 12 Hrs

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

(III) Transition Metal π -Complexes 18 Hrs

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

(IV) Transition Metal Compounds with Bonds to Hydrogen 3 Hrs

Transition metal compounds with bonds to hydrogen.

(V) 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 olefins (oxo reaction), oxopalladation reaction, activation of C-H bond.

(VI) Fluxional Organometallic Compounds 8 Hrs

Fluxional and dynamic equilibria in compounds such as η^2 - olefin, η^3 - allyl and dienyl complexes.

Books Suggested

1. Principles and Application of Organotransition Metal Chemistry, J. P. Collman, L. S. Heagsdus, J. R. Norton and R. G. Finke, University Science Books.
2. The Organometallic Chemistry of 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.

PAPER-IV: MCHE-304

Inorganic Chemistry (Analytical & Coordination Chemistry)

60 Hrs

(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) Analysis of Water Pollution

15 Hrs

Origin of waste 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 and analysis. Water laws and standards.

(IV) Structures of 2 to 8 Coordinate Metal Complexes

15 Hrs

Cation-anion ratio in various polyhedral, Hybrid orbitals and preferred conditions of formation of the complexes of following geometries:

- Linear
- Trigonal planar, Trigonal pyramidal

- Tetrahedral, Square planar
- Trigonal bipyramidal, Square pyramidal, pentagonal.
- Octahedral, Trigonal prism
- Pentagonal bipyramidal, Capped octahedral, Capped trigonal prism.
- Cubic, Tetragonal antiprismatic, Dodecahedral, Hexagonal bipyramidal, and Bicappedtrigonal prism,
Stereochemical non-rigidity in four to eight coordinate Complexes.

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.
11. Inorganic Chemistry, 4th Edition, Principles of Structure and Relativity by J.E. Huheey, E.A. Keiter and R.L. Keiter, 1993.
12. Chemistry of Elements by N.N. Greenwood and A. Earnshaw, Butterworths, 1997.
13. Mechanism of Inorganic Reactions; A Study Of Metal Complexes in Solution by F. Bosolo and R.G. Pearson.
14. Ligand Field Theory And Its Application by B.N. Figgis and M.A. Hitchman, Wiley, New York, 2000.

PAPER-III: MCHE-305

Organic Chemistry (Organic Synthesis-I)

60 Hrs

(a) Organometallic Reagents

25 Hrs

Principle, preparations, properties and application of the following in organic synthesis with mechanistic details

Group I and II metal organic compounds

Li, Mg, Hg, Cd, Zn and Ce compounds

Transition metals

Cu, Pd, Ni, Fe, Co, Rh, Cr and Ti Compounds

(b)Oxidation

10 Hrs

Introduction. Different oxidative processes. Hydrocarbons-alkenes, aromatic rings, saturated C-H groups (activated and unactivated). Alcohols, diols, aldehydes, and sulphides. Amines, hydrazines, and sulphides. Oxidations with ruthenium tetroxide, iodobenzene diacetate.

(c)Reduction

10 Hrs

Introduction. Different reductive processes. Hydrocarbons-alkanes, alkenes, alkynes and aromatic rings. Carbonyl compounds-aldehydes, ketones, acids and their derivatives, Epoxides. Nitro, nitroso, azo and oxime groups. Hydrogenolysis.

(d)Rearrangements

15 Hrs

General mechanistic considerations – nature of migration, migratory aptitude, memory effects. A detailed study of the following rearrangements Pinacol-pinacolone, Wagner-Meerwein, Demjanov, Benzil Benzilic acid, Favorskii, Arndt Eistert synthesis, Neber, Beckmann, Hoffmann, Curtius, Schmidt, Baeyer-Villiger, Shapiro reaction.

Books Suggested

1. Modern Synthetic Reactions, H.O. House, W.A. Benjamin.
2. Some modern Methods of organic Synthesis, W. Carruthers Univ. Press.

3. Advanced Organic Chemistry, Reactions Mechanisms and Structure, J. March, John Wiley.
4. Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, Blackie Academic & Professional.
5. Advanced Organic Chemistry Part B, F.A. Carey and R.J. Sundberg. Plenum Press.
6. Rodd's Chemistry of Carbon Compounds Ed. S. Coffey, Elsevier.
7. Advanced Organic Chemistry, Jagdamba Singh, L. D. S. Yadav, A Pragati Edition.

PAPER-IV: MCHE-306

Chemistry of Heterocyclic Compounds and Photochemistry 60 Hrs

Unit-I: Heterocyclic Chemistry 30 Hrs

(I) Nomenclature of Heterocyclic and their synthesis 8 Hrs

Replacement and systematic nomenclature (Hantzsch-Widman system) for monocyclic, fused and bridged heterocycles. Principles of heterocyclic synthesis involving cyclization reaction and cycloaddition reaction.

(II) Small Ring Heterocycles 8 Hrs

Three-membered and four-membered heterocycles-synthesis and reactions of aziridines, oxiranes, thiranes, azetidines, oxetanes and thietanes.

(III) Benzo-Fused Five-Membered Heterocycle 6 Hrs

Synthesis and reaction including medicinal application of benzopyrroles. Benzofurans and benzothiophenes.

(IV) Six-Membered Heterocycles with One Heteroatom 8 Hrs

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

Unit-II: Photochemistry 30 Hrs

(I) Photochemical Reactions 5 Hrs

Interaction of electromagnetic radiation with matter, types of excitations, fate of excited molecule, quantum yield, transfer of excitation energy, actinometry.

(II) Photochemistry of Alkenes and Carbonyl Compounds **15 Hrs**

Intramolecular reactions of the olefinic bond – geometrical isomerism, cyclisation reactions, rearrangement of 1, 4- and 1, 5-dienes. Intramolecular reactions of carbonyl compounds – saturated, cyclic and acyclic, β , γ – unsaturated and α , β – unsaturated compounds. Cyclohexadienones. Intermolecular cycloaddition reaction – dimerisations and oxetane formation.

(III) Photochemistry of Aromatic Compounds **4 Hrs**

Isomerisations, additions and substitutions.

(IV) Miscellaneous Photochemical Reactions **6 Hrs**

Photo-Fries reaction of anilides. Photo-Fries rearrangement. Barton reaction. Photochemistry formation of smog. Photodegradation of polymers. Photochemistry of vision.

Books Suggested

1. Heterocyclic Chemistry Vol.1-3, R.R. Gupta. M. Kumar and V.Gupta, Springer Verlag.
2. The chemistry of Heterocycles, 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 Gilchrist, Longman Scientific Technical.
5. Contemporary Heterocyclic Chemistry, G.R. Newkome and W.W. Paudler, Wiley-Inter Science.
6. An Introduction to the Heterocyclic Compounds, R.M. Acheson, John Wiley.
7. Comprehensive Heterocyclic Chemistry, A.R. Katritzky and C. W. Rees, eds, Pergamon Press.
8. Fundamentals of Photochemistry, K.K. Rohtagi-Mukherji, Wiley-Eastern
9. Essentials of Molecular Photochemistry, A.Gilbert and J.Baggott, Blackwell Scientific Publication.
10. Photochemistry, R.P. Kundall and A.Gilbert, Thomson Nelson.
11. Organic Photochemistry, J.Coxon and B.Halton, Cambridge University Press.

PAPER -III: MCHE-307

Chemistry of Material **60 Hrs**

(I) Multiphase Materials **6Hrs**

Ferrous alloys; Fe-C phase transformation in ferrous alloys; stainless steels, non-ferrous, properties of ferrous and non-ferrous alloys and their applications.

(II) Glasses, Ceramics, Composites And Nanomaterials**14Hrs**

Glassy state, glass formers and glass modifiers, applications. Ceramic structures, mechanical properties, clay products. Refractories, characterization, properties and applications. Microscopic composites; dispersion-strengthened and particle-reinforced fibre-reinforced composites, macroscopic composites Nanocrystalline phase, preparation procedures, special properties, applications.

(III) Liquid Crystals**15Hrs**

Mesomorphic behaviour liquid crystals, positional order, bond orientational order, nematic and smectic mesophases; smectic-nematic transition and clearing temperature-homeotropic, planar and schlieren textures, twisted nematics, chiral nematics, molecular arrangement in smectic C phase, optical properties of liquid crystals. Dielectric susceptibility and dielectric constants. Lyotropic phase and their description of ordering in liquid crystals.

(IV) Ionic Conductors**10Hrs**

Types of ionic conductors, mechanism of ionic conductors, interstitial jumps (Frenkel); vacancy mechanism, diffusion, superionic conductors; phase transitions and mechanism of conduction of superionic conductors, examples and applications of ionic conductors.

(V) Organic Solids, Fullerenes, Molecular Devices**15Hrs**

Conducting organics, organic superconductors, magnetism in organic materials. Fullerenes-doped, fullerenes as superconductors. Memory and switches-sensors. Nonlinear optical materials: nonlinear optical effects, second and third order-molecular hyper polarisability and second order electric susceptibility materials for second and third harmonic generation.

Books Suggested:

1. Solid State Physics, N.W. Ashcroft and N.D. Mermin, Saunders College.
2. Material Science and Engineering, An Introduction, W.D., Callister, Wiley.
3. Principles of the Solid State, H.V. Keer, Wiley Eastern
4. Materials Science, J.C. Anderson, K.D. Leaver, J.M. Alexander and R.D. Rawlings, ELBS.
5. Thermotropic Liquid Crystals, Ed., G.W. Gray, John Wiley.
6. Handbook of Liquid Crystals, Kelker and Hatz, Chemie Verla

PAPER – IV MCHE-308**Statistical Thermodynamics and Chemical Dynamics****60 Hrs****Unit-I: Statistical Thermodynamics****30 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, calculations of thermodynamic properties in terms of partition functions. Application of partition functions. Heat capacity behaviour of solids- chemical equilibria and equilibrium constant in terms of partition functions, Fermi- Dirac statistics, distribution law and applications to metal Bose- Einstein statistics- distribution law and application to helium.

Unit-II: Chemical Dynamics

30 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 (Belousav- Zhabotinsky reaction), homogeneous catalysis kinetics of enzyme reactions, general features of fast reactions, study of fast reactions by flow method, relaxations method, flash photolysis and the nuclear magnetic resonance method. Dynamic 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).

Solid State : Thermodynamics of Schottky and Frankel Defects, Solid State Reaction.

Books Suggested

1. Physical Chemistry, P.W. Atkins, ELBS.
2. Chemical Kinetics, K.L. Laidier, McGraw- Hill.
3. Kinetics and Mechanism of Chemical Transformation, J. Rajaraman and J.Kuriacose, McMillan.
4. Micelles, Theoretical and Applied Aspects, V. Morol, Plenum.

PAPER-VI: MCHP 309

PRACTICAL / LAB

Time Duration: 12 Hours in two days (Max Marks: 100 (EACH))

MCHP -309 (A) Inorganic chemistry exercise (Specialization in Inorganic Chemistry)

- 1 – EDTA Titration- Zn, Ca, Mg, Fe.
- 2 – Idimetric and Idometric titrations from copper sulphate.
- 3- Determination of Na & K by Flame Photometry
- 4- Synthesis and characterization of Schiff's Base and its transition metal complexes on the basis of available physico-chemical and spectral methods.

MCHP -309 (B) Organic chemistry exercise (Specialization in Organic Chemistry)

- A – Determination of percentage of Hydroxyl group.
- B – Purification of compound by
Steam distillation, Fractional distillation. Distillation under reduce pressure, crystallization.
- C – Chromatographic studies of sugar by determine RF value
- D – Saponification value, Iodine value

MCHP -309 (C) Physical chemistry exercise (Specialization in Physical Chemistry)

- 1 –Determination of partial molar volumes of a salt and water for aqueous solutions at room temperature.
- 2- Determination of specified volume and molar volume of a given liquid at room temperature.
- 3 – Adsorption of oxalic acid on activated charcoal and to verify Langmuir's theory.
- 4 –Determination of the strength of strong acid & weak acid in given mixture conductrometric.
- 5 – Determination of molecular weight of a given substance using water as the solvent by Landsbergis method

PAPER-VII: MCHP 310
DISSERTATION / PROJECT

Semester IV

PAPER- I: MCHC-401

SPECTROSCOPY-II **60 Hrs**

1. Mass Spectrometry **15 Hrs**

Measurement technique (EI, CI, FD and FAB), Molecular base and molecular ions, various class of organic molecules, McLafferty re-Arrangement and retro-Diels-Alder Fragmentation, nitrogen rule and determination of molecular composition of organic compounds from mass spectra data.

2. Nuclear magnetic resonance **25 Hrs**

(A). ^1H NMR: The spinning nuclei, Chemical shift and its measurement, factors affecting chemical shifts, anisotropic effect and shielding mechanism, interpretation of protons spin-spin coupling, coupling constant, Chemical and magnetic equivalence, first and non-first order spectra, Simplification of complex spectra and NOE deuterium exchange, application in structural determination of simple organic. (B). ^{13}C NMR: General introduction, peak assignments, chemical shift, $^{13}\text{C}^1\text{H}$ coupling, Off-resonance Decoupling, Deuterium, fluorine and phosphorus coupling, NOE and DEPT, 2D NMR: COSY, and HETCOR, Application to simple organic.

3. Electron Spin Resonance Spectroscopy **10 Hrs**

Basic principle, factor affecting value, isotropic and anisotropic hyperfine coupling constant, Application to organic free radical, Methyl Free Radical, Naphthalene and Benzene free radicals.

4. Mossbauer Spectroscopy **10 Hrs**

Theory, Instrumentation, Applications - isomer shift, nuclear quadruple coupling and hyperfine

interaction, Problems related to Mossbauer Spectroscopy.

Books Suggested

1. Structural Methods in inorganic Chemistry, E.A.V. Ebsworth, D.W.H. Rankin and S. Cradock, ELBS.
2. Infrared and raman Spectra: Inorganic and Coordination Compounds, K.Nakamoto, Wiley.
3. Progress in inorganic Chemistry vol., 8 ed., F.A. Cotton, vol., 15, ed. S.J. Lippard, Wiley.
4. Transition Metal Chemistry ed. R.L. Carlin vol. 3. Dekker.
5. Inorganic Electronic Spectroscopy, A.P.B. Lever, Elsevier.
6. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R.V. Parish, Ellis Horwood.
7. Practical NMR Spectroscopy, M.L., J.J. Delpeuch and G.J. Sassler and T.C. Morrill, John Wiley.
8. Spectrometric Identification of Organic Compounds, R.M. Silverstein, G.C. Bassler and T.C. Morrill, John Wiley.
9. Introduction to NMR Spectroscopy, R.J. Abraham, J. Fisher and P.Loftus. Wiley.
10. Application of Spectroscopy of Organic compounds, J.R. Dyer, Prentice Hall.
11. Spectroscopic Methods in Organic Chemistry, D.H. Williams, I. Fleming. Tata McGraw-Hi.
12. Physical Methods for Chemistry, R.S. Drago, Saunders Company.

PAPER-II MCHC-402

Green Chemistry

60 Hrs

Unit I Introduction

12Hrs

Introduction-Current status of chemistry and the Environment-Evolution of the Environmental movement: Public awareness - Dilution is the solution to pollutionPollution prevention

Unit II Principles

12Hrs

Green Chemistry – Definition – Principles of Green Chemistry - Why is this new area of Chemistry getting to much attention - Why should chemist pursue the Goals of Green Chemistry - The roots of innovation – Limitations

Unit III Bio Catalytic Reactions

12Hrs

Green Chemistry Using Bio Catalytic Reactions – Introduction - Fermentation and Bio transformations - Production of Bulk and fine chemicals by microbial fermentationAntibiotics – Vitamins - Bio catalyses synthesis of industrial chemicals by bacterial constructs - Future Trends.

Unit IV Green House Effect

12Hrs

Green house effect and Global Warming – Introduction - How the green house effect is produced - Major sources of green house gases - Emissions of CO₂ - Impact of green house effect on global climate - Control and remedial measures of green house effect - Global warming a serious threat - Important points.

Unit V Green Analytical Methods

12Hrs

Future trends in Green Chemistry - Green analytical methods, Redox reagents, Green catalysts; Green nano-synthesis, Green polymer chemistry, Exploring nature, Biomimetic, Proliferation of solvent-less reactions; Non-covalent derivatization, Biomass conversion, emission control.

Books Suggested

1. V. Kumar, "An Introduction to Green Chemistry" Vishal publishing Co. Reprint Edition 2010.
2. Rashmi Sanghi, M.M Srivastava "Green Chemistry" Fourth Reprint – 2009

PAPER- III: MCHC-403

Inorganic Chemistry (Photo Inorganic & Supramolecular Chemistry)

60 Hrs

(I) Basics of Photochemistry

10 Hrs

Absorption, excitation, photochemical laws, quantum yield, electronically excited states life times-measurements of the times. Flash photolysis, stopped flow techniques. Energy dissipation by radiative and non-radiative processes, absorption spectra, Franck-Condon principle, photochemical stages-primary and secondary processes.

(II) Excited States of Metal Complexes

8 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.

(III) Ligand Field Photochemistry

8 Hrs

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

(IV) Supramolecular Chemistry

18 Hrs

Concepts and language.

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

(B) Supramolecular reactivity and catalysis.

(C) Transport processes and carrier design.

Books Suggested

1. 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., 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.

PAPER- IV: MCHC-404

Inorganic Chemistry (Bioinorganic Chemistry) 60 Hrs

(I) Metal Storage Transport and Biomineralization 5 Hrs

Ferritin, transferrin, and siderophores

(II) Calcium in Biology 6 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 oxotransferase enzymes – xanthine oxidase. Conenzyme vitamin B₁₂.

(IV) Metal – Nucleic Acid Interactions 6 Hrs

Metal ions and metal complex interactions. Metal complexes – nucleic acids

(V) Metals in Medicine 5 Hrs

Metal deficiency and disease, toxic effects of metals, metals used for diagnosis and

chemotherapy with particular reference to anticancer drugs.

Books Suggested

1. Principles of Bioinorganic Chemistry, S.J.Lippard and J.M. Berg, University 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 38 ed. J.J. Lippard, Wiley
5. Supramolecular Chemistry, J.M. Lehn, VCH.

PAPER-III MCHE-405

Organic Chemistry (Organic Synthesis- II) 60 Hrs

(I) Disconnection Approach 20 Hrs

An introduction to synthons and synthetic equivalents, disconnection approach, functional group inter-conversions, the importance of the order of events in organic synthesis, one group C-X and two group C-X disconnections, chemoselectivity, reversal of polarity, cyclization reactions, amine synthesis.

(II) Protecting Groups 8 Hrs

Principle of protection of alcohol, amine, carbonyl and carboxyl groups.

(III) One Group C-C Disconnection 10 Hrs

Alcohols and carbonyl compounds, regioselectivity. Alkene synthesis, use of acetylenes and aliphatic nitro compounds in organic synthesis.

(IV) Two Group C-C Disconnections 12 Hrs

Diels-Alder reaction, 1,3-difunctionalised compounds, α , β – unsaturated carbonyl compounds, control in carbonyl condensations, 1,5- difunctionalised compounds. Micheal addition and Robinson annelation.

(V) Ring Synthesis 10 Hrs

Saturated heterocycles, synthesis of 3-, 4-, 5- and 6-membered rings, aromatic heterocycles in

organic synthesis.

Books Suggested

1. Designing Organic Synthesis, S. Warren, Wiley.
2. Organic Synthesis-Concept, Methods and Starting Materials, J.Fuhrhop and G.Penzilin, Verlage VCH.
3. Some Modern Methods of Organic Synthesis. W. Carruthers, Cambridge Univ. Press.
4. Modern Synthetic Reactions, H.O. House, W.A. Benjamin.
5. Advanced Organic Chemistry: Reactions, Mechanisms and Structure, J. March, Wiley.
6. Principles of Organic Synthesis, R.Norman and J.M.Coxon, Blackie Academic & Professional.
7. Advanced Organic Chemistry Part B, F.A. Carey and R.J.Sundberg, Plenum Press.

PAPER-IV: MCHE-406

Organic Chemistry (Chemistry of Natural Products) 60 Hrs

(I) Terpenoids and Carotenoids 20 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 – Terperneol, Menthol, Farnesol, Zingiberene, Camphor, Phytol, Abietic acid and β –Carotene.

(II) Alkaloid 20 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: Ephedrine, Conine, Atropine, Nicotine, Quinine, Morphine.

(III) Steroids 14 Hrs

Occurrence, nomenclature, basis skeleton, Diel's hydrocarbon and stereochemistry. Cholesterol, Sex harmones (Androgens and Estrogens). Biosynthesis of steroids.

(IV) Porphyrins 6 Hrs

Structure and synthesis of Haemoglobin and Chlorophyll.

Books Suggested

1. Natural Products: Chemistry and Biological Significance, J.Mann. R.S.Davidson, J.B.Hobbs, V. Banthrope and J.B. Harborne. Longman, Essex.
2. Organic Chemistry, Vol 2, I.L. Finar, ELBS.
3. Stereoselective Synthesis: A Practical Approach, M. Nogradi, VCH.
4. Rodd's Chemistry of Carbon Compounds, Ed. S. Coffey, Elsevier.
5. Chemistry, Biological and Pharmacological Properties of Medicinal Plants from the Americas, Ed. Kurt Hostettmann. M. P. Gupta and A. Marston. Harwood Academic Publishers.
6. Introduction to Flavonoids, B.A. Bohm, Harwood Academic Publishers.
7. New Trends in Natural Product: Chemistry, Atta-ur-Rahman and M.I. Choudhary, Harwood Academic Publishers. Insecticides of Natural Origin, Sukh Dev, Harwood Academic Publishers.

Paper-III: MCHE-407

Physical Chemistry (Advanced Quantum Chemistry) 60 Hrs

Unit-1 Huckel Molecular Orbital Theory and its Applications: 15 Hrs

Calculation of π -energy levels and delocalisation energy of butadiene, cyclic conjugated polyolefins - cyclopropenyl, cyclobutadiene, cyclopentadienyl, benzene, tropylium radical and cyclooctatetraene, concept of aromaticity and antiaromaticity, Huckel treatment of linear polyenes

Unit-2 Semi-Empirical and Ab-Initio SCF Theories: 15 Hrs

Hartree-Fock Self consistent field (SCF) method, Semi-empirical SCF theory (CNDO, INDO & MNDO), Slater and Gaussian type orbitals, configuration interaction and electron correlation, Moeller- Plasset Perturbation methods, Introduction to molecular mechanics.

Unit-3 Introduction to density functional theory: 13 Hrs

Concept of basic sets, exchange-correlation energy and Kohn-Sham orbitals, Local Density Approximation (LDA) and Generalized Gradient Approximation (GGA), Significance of Density Functional Theory.

Unit-4 Thermodynamics of Irreversible Processes: 17 Hrs

Entropy production in irreversible processes, Entropy equation for heat flow, relation between fluxes and forces, Non-equilibrium stationary states, linear phenomenological equations, Onsager's reciprocity relation, non-linear thermodynamics treatment of electro-kinetic phenomena, thermo-osmosis and reverse osmosis, Intermolecular Forces: Dispersion, dipole, induction and Charge transfer forces. The hydrogen bond.

Books Recommended:

1. Chemical Application of Group Theory – F.A. Cotton.
2. Introductory Quantum Chemistry – A.K. Chandra.
3. An Introduction to Quantum Mechanics of Chemical Systems – R.P. Rastogi and V.K. Srivastava.
4. Physical Chemistry – P.W. Atkins.
5. Valence Theory – J.N. Murrell, S.F.A. Kettle and J.M. Teddor.
6. Chemistry by Ira N. Levine Prentice Hall of India New Delhi 1995.
7. Coulson's volume by R. McWeeny ELBS 1978.

Paper-IV: MCHE-408

Physical Chemistry (Polymer Chemistry)

60 Hrs

(I) Basics

8 Hrs

Importance of polymers. Basic concepts: Monomers, repeat units, degree of polymerization Linear, branched and network polymers. Classification of polymers. Polymerization: condensation, addition, radical chain-ionic and co-ordination and co-polymerization. Polymerization conditions and polymer reactions. Polymerization in homogeneous and heterogeneous systems.

(II) Polymer Characterization

14 Hrs

Polydispersion-average molecular weight concept. Number, weight and viscosity average molecular weights. Polydispersity and molecular weight distribution. The practical significance of molecular weight. Measurement of molecular weight. End-group, viscosity. Light scattering, osmotic and ultracentrifugation methods. Analysis and testing of polymers chemical analysis of polymers. Spectroscopic methods. X-ray diffraction study. Microscopy. Thermal analysis and physical testing-tensile strength. Fatigue, impact. Tear resistance. Hardness and abrasion resistance.

(III) Structure and Properties

14 Hrs

Morphology and order in crystalline polymers-configuration of polymer chains. Crystal structures of polymers. Morphology of crystalline polymers, strain-induced morphology, crystallization and melting. Polymer structure and physical properties-crystalline melting point T_m – melting points of homogeneous series, effect of chain flexibility and other steric factors, entropy and heat of fusion. The glass transition temperature, Relationship between T_m and T_g . Effects of molecular weight. Diluents, chemical structure, chain topology, branching and cross linking. Property requirements and polymer utilization.

(IV) Polymer Processing

12 Hrs

Plastic, elastomers and fibres, compounding. Processing techniques: Calendering, die casting, rotational casting, film casting, Injection moulding, blow moulding, extrusion moulding, thermoforming, foaming, reinforcing and fibre spinning.

(V) Properties of Commercial Polymers

2 1Hrs

Polyethylene, polyvinyl chloride. Polyesters, phenolic resins, epoxy resin and silicone polymers. Functional polymers – fire retarding polymers and electrically conducting polymers. Biomedical polymers – contact lens, dental polymers, artificial heart, kidney, skin and blood cells.

Books Suggested

1. Textbook of Polymer Science, F.W. Billmeyer Jr. Wiley.
2. Polymer Science, V.R. Gowariker, N.V. Viswanathan and J. Sreedhar, Wiley-Eastern.
3. Functional Monomers and Polymers, K. Takemoto, Y. Inaki and R.M. Otanbrite.
4. Contemporary Polymer Chemistry, H.R. Alcock and F.W. Lambe Prentice Hall.

Paper-VI: MHCP-409

PRACTICAL / LAB

Time Duration: 12 Hours in two days

(Max Marks: 100 (EACH))

MCHP -409 (A) Inorganic chemistry exercise (Specialization in Inorganic Chemistry)

- 1 – Qualitative analysis of mixture of eight radicals including at least two rare earth metal
- 2 – Gravimetric and volumetric estimation of three metal ions (Ag, Cu, Ni) (Fe, Ni, Zn)
- 3 – Colorimetry & Spectro photometry estimation of following metals in solutions V, Cr, Fe, Ni.

- 4 – Analysis of ores, minerals and alloys
- a – Analysis of Iron In the given iron ore solution
- b – Analysis of Brass
- c – Analysis of Silver coin

MCHP -409 (B) Organic chemistry exercise (Specialization in Organic Chemistry)

- A – Three step preparation of organic compounds.
- B – Organic mixture analysis for three components.
- C – U.V. Spectro photometric estimation of
Amino acids, Proteins, Caffeine, Aspirin
- D (1) – Condensation reaction
(a) Aldol (b) Knoevenagel reaction
- D (2) – Cannizaro reaction

MCHP -409 (C) Physical chemistry exercise (Specialization in Physical Chemistry)

- 1 –Determination of specific and molar rotation of an optically active substance by polar meter measurement
- 2- Determination of refractive index of a given liquid by abbe refractometer
- 3 – Determination of strength of unknown solution of HCl titrating it with NaOH Solution using PH meter.
- 4 –Determination of composition of a mixture by conductometry.

Paper-VII: MHCP-410

DISSERTATION/ PROJECT