M. J. P. ROHILKHAND UNIVERSITY, BAREILLY

महात्मा ज्योतिबा फुले
रुहेलखण्ड विश्वविद्यालय, बरेली

CHEMISTRY POST GRADUATE SYLLABUS

SEMESTER SYSTEM

STARTING FROM 2022-2023

BY

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महात्मा ज्योतिबा फुले रूहेलखण्ड विश्वविद्यालय, बरेली
MAHATMA JYOTIBA PHULE ROHILKHAND UNIVERSITY, BAREILLY

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कार्यालय ज्ञाप

रसायन विज्ञान पाठ्य समिति के संयोजक का कार्यकाल समाप्त होने के उपरान्त वरिष्ठता चक्रानुक्रम में नवीन संयोजक का गठन निम्नवत् किया गया है।

1. डा0 शची मित्तल — संयोजक
   बरेली कालेज, बरेली
2. डा0 आदित्य कुमार मिश्रा — सदस्य
   एन0 एम0 एस0 एन0 दास कालेज, बदायूं
3. दिव्या सिंह — सदस्य
   बरेली कालेज, बरेली
4. डा0 शोभा गुप्ता — सदस्य
   डी0 ए0 के0 कोलज, मुरादाबाद
5. डा0 एन0 बी0 सिंह — सदस्य
   बरेली कालेज, बरेली
6. डा0 डी0 पी0 सिंह — बाह्य विशेषज्ञ
   एन0 आई0 टी0, कुरूक्षेत्र
7. प्रो0 दिनेश मोहन — बाह्य विशेषज्ञ
   पर्यावरण विज्ञान विभाग, जे0एन0यू0, नई दिल्ली

भवदीय

कुलसचिव

प्रतिलिपि– निम्नलिखित को सूचनार्थ एवं आवश्यक कार्यवाही हेतु प्रेषित।

1. सम्बन्धित सदस्य / बाह्य विशेषज्ञ।
2. निजी सचिव, कुलपति को कुलपति महोदय के सूचनार्थ।

कुलसचिव

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 16 credits in one semester. Lab exercises would comprise of 6 credits in each of first two semesters. In addition, there will be 2 credits for seminar presentation in each of first two semesters.

Minor/Open elective paper:

- Student will also have to study a Minor elective paper in first / second semester of post graduate program.
- This minor elective paper could be selected from the available paper of subjects running in the institution.
- Minor Elective paper will be different from Major Subject. This paper will be of 4 credits.
- In general, colleges should schedule classes of minor subjects in time table. The internal assessment of minor subject will also be held along with semester exam as decided by University.
- 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 semester which would be evaluated in the last semester.
- This research project may be interdisciplinary/ multidisciplinary. Itmay 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 would comprise of 16 credits out of which 8 credits for project compilation and successful submission. Remaining 8 credits will be awarded by evaluation committee.

- **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 52 credits in Ist year and 48 credits in IInd year. The division of credits will be as follows:

I year (52 credits)

I semester-

- 4x4= 16 credits for core papers
- 6 credits for Lab work
- 2 credits for seminar
- **Total 24 credits**

II semester-

- 4x4= 16 credits for core papers
- 4 credits for minor paper
- 6 credits for Lab work
- 2 credits for seminar
- **Total 28 credits**

II year (48 credits)

III semester-

- 2x4= 8 credits for core papers
- 2x4= 8 credits for elective papers
- 8 credits for Dissertation/Project
- **Total 24 credits**

IV semester-

- 2x4= 8 credits for core papers
- 2x4= 8 credits for elective papers
- 8 credits for Dissertation/Project
- **Total 24 credits**

- **Thus, in total there are 52+48 = 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 excluding research project.
- All the Major and minor subjects will be evaluated externally and internally both.
- Out of 100 max. marks, 25 marks will be awarded for internal evaluation and 75 marks for external evaluation.
- For internal evaluation, a written test of 10 marks will be conducted. 10 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 both semesters, the prepared project report/dissertation will be evaluated by external and internal examiners in 50 marks separately. The student will be evaluated for 50 marks on the basis of concerned viva-voce/ presentation from his research project.

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**
MCHC-102	**PAPER- II**	**Organic Chemistry**	**4/100**
MCHC-103	**PAPER- III**	**Physical Chemistry**	**4/100**
MCHC-104	**PAPER- IV**	**Group Theory**	**4/100**
MCHL-105	**PAPER- V**	**Practical & Seminar**	**8/200**
			Total =24/600

SEMESTER –II			
COURSE CODE	**PAPER NUMBER**	**PAPER NAME**	**CREDIT/MAX. MARKS**
MCHC-201	**PAPER- I**	**Inorganic Chemistry**	**4/100**
MCHC-202	**PAPER- II**	**Organic Chemistry**	**4/100**
MCHC-203	**PAPER- III**	**Physical Chemistry**	**4/100**

MCHC-204	**PAPER- IV**	**Instrumental Chemistry**	**4/100**
MCHM-205	**PAPER- V**	**Minor**	**4/100**
MCHL-206	**PAPER- VI**	**Practical & Seminar**	**8/200**
			Total =28/700

SEMESTER –III				
COURSE CODE	**PAPER NUMBER**	**PAPER NAME**	**PAPER TITLE**	**CREDIT/ MAX. MARKS**
MCHC-301	**PAPER- I**	**Spectroscopy**	**Spectroscopy-1**	**4/100**
MCHC-302	**PAPER- II**	**Recent Trends**	**Recent Trends in Chemistry**	**4/100**
MCHE-303	**PAPER- III**	**Inorganic Chemistry**	**Organotransition Metal Chemistry**	**4/100**
MCHE-304	**PAPER- IV**	**Inorganic Chemistry**	**Analytical & Coordination Chemistry**	**4/100**
MCHE-305	**PAPER- III**	**Organic Chemistry**	**Organic Synthesis-1**	**4/100**
MCHE-306	**PAPER- IV**	**Organic chemistry**	**Heterocyclic Compounds & Photo chemistry**	**4/100**
MCHE-307	**PAPER- III**	**Physical Chemistry**	**Chemistry of Material**	**4/100**
MCHE-308	**PAPER- IV**	**Physical Chemistry**	**Liquid State**	**4/100**
MCHP-309	**PAPER - V**	**Dissertation/ Project**	**Research Work**	**8/000**
				Total =24/400

SEMESTER-IV				
COURSE CODE	**PAPER NUMBER**	**PAPER NAME**	**PAPER TITLE**	**CREDIT/ MAX. MARKS**
MCHC-401	**PAPER I**	**Spectroscopy**	**Spectroscopy-II**	**4/100**

MCHC-402	**PAPER II**	**Green Chemistry**	**Green Chemistry**	**4/100**
MCHE-403	**PAPER III**	**Inorganic Chemistry**	**Photo Inorganic &supramolecular Chemistry**	**4/100**
MCHE-404	**PAPER IV**	**Inorganic Chemistry**	**Bioinorganic Chemistry**	**4/100**
MCHE-405	**PAPER III**	**Organic Chemistry**	**Organic Synthesis- II**	**4/100**
MCHE-406	**PAPER IV**	**Organic Chemistry**	**Chemistry of Natural Product**	**4/100**
MCHE-407	**PAPER III**	**Physical Chemistry**	**Advanced Quantum Chemistry**	**4/100**
MCHE-408	**PAPER IV**	**Physical Chemistry**	**Polymer Chemistry**	**4/100**
MCHP-409	**PAPER V**	**Dissertation/ Project**	**Research Work**	**8/100**
				Total 24/500

Abbreviations:

MCHC : M.Sc. Chemistry Core paper

MCHL :M.Sc. Chemistry Lab

MCHM : M.Sc. Chemistry Minor elective

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,M,L,P,E) : Nature of course

(C: Core paper, M: Minor elective, 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) dπ - pπ 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 Equililbria 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. Earnshow, 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 enegy relationship, subsituent and reaction constants.

(III) Aliphatic Nucleophilic Substitution **12 Hrs**

The SN_2, SN_1, mixed SN_1 and SN_2 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 SN_{Ar}, SN_1 benzyne and SRN_1 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, Vilsmeir 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. Reactvity in the attacking radicals. The effect of solvents on reactivity. Allylic halogenation (NBS) oxidation of aldehydes to carboxlic 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 explicity). 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. McGarw Hill.
5. DM Bishop, “Group Theory and Chemistry” Dover Publication.

PAPER – V: MCHL-105

Ist SEM. PRACTICAL

Inorganic Chemistry Exercise

1. Qualitative analysis of Inorganic mixture containing seven radicals including

(i) Rare earth elements (ii) Anions, which have not been done in under graduate practical (iii) Insoluble.

2. Separation of cations by following chromatographic techniques:

- Paper chromatography
- Column chromatography
- Ion Exchange Chromatography

3. Conductometric titration of

Strong acid against strong base

Strong acid against weak base

Organic Chemistry Exercise

1. Separation, Purification and Identification of compounds of three component mixture
2. Organic Synthesis

- Oxidation (as sugar to oxalic acid)
- Nitration (as Nitrobenzene to m-dinitrobenzene)
- Acetylation (as Salicylic acid to aspirin)
- Sandmeyer reaction (as p-toluedine to p-chloro toluedine)
- Grignard reaction (as benzoic acid to phenyl methanol)

Physical Chemistry Exercise

1- Error analysis and statistical data analysis.

2- Study surface tension concentration relationship of two solutions.

3- Determine adsorption of oxalic acid and activated charcoal to verify Langmuir's theory.

4- Determine the heat of solution of $CuSO_4.5H_2O$ solution.

5- Determination of pH by following method.
(a) Electrical Conductivity method (b) Polarography

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

Marks Distribution for Lab. Course for M.Sc. 1st Semester

(a) Inorganic Chemistry Exercise: **40 Marks**

(b) Organic Chemistry Exercise: **40 Marks**

(c) Physical Chemistry Exercise: **40 Marks**

(d) Attendance + Record + Viva: **30 Marks**

(e) Seminar : **50 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, metalloborances 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. Earnshow, 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. Witting 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 E_2, E_1, 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- butadience, 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. Cycloaddditions- antarafacial and suprafacial additions, 4n and 4n+2 systems, 2+2 addition of ketenes, 1,3 dipolar cycloadditions and cheleotropic 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, Mecmilan, 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, llkovic 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: MCHC-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 oxidationreduction and acid-base titrations, comparison with the conductometric method.

(c) **Voltammetry:** Cyclic voltammetry

(d) **Polarography:** Dropping mercury electrons 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 $CaC_2O_4.H_2O$ and $MgC_2O_4.2H_2O$

(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

(b) 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

Minor Paper

PAPER-V: MCHM-205

Environmental Chemistry (For all students)

General Concept of Environmental Sciences **30 Hrs**

UNIT I **8 Hrs**

Composition of atmosphere, vertical and horizontal distribution of temperature, Relationship of earth with sun,

UNIT II **10 Hrs**

Global warming, Ozone hole, Western disturbances, EI-nino, La-nino, Green house gases and their effects , Environmental ethics, History of climate change.

UNIT III **12 Hrs**

Definition, principles and scope of ecology, human ecology and human settlements, evolution, origin of life and specification, Ecosystem stability-cybernatics and ecosystem regulation, evolution of biosphere.

Mathematics for Chemists (For Bio Students in B.Sc) **30 Hrs**

UNIT I Vectors and Matrix Algebra **10 Hrs**

(A) Vectors

Vectors, dot, cross and triple products etc. The gradient, divergence and curl. Vector calculus, Gauss' theorem, divergence theorem etc.

(B) Matrix Algebra

Addition and multiplication, inverse, adjoint and transpose of matrices, special matrices (Symmetric, Skew-symmetric, Hermitian, SkewHermitian, unit, diagonal, unitary etc.) and their properties. Matrix equation : Homogeneous, non-homogeneous linear equations and conditions for the solution, linear dependence and independence. Introduction to vector spaces matrix

eigenvalues and eigenvectors, diagonalization, determinants (examples from Huckel theory). Introduction to tensors; polarizability and magnetic susceptibility as examples.

UNIT II Differential Calculus **10 Hrs**

Functions, continuity and differentiability, rules for differentiation application of differential calculus including maxima and minima (examples related to maximally populated rotational energy levels, Bohr's radius and most probable velocity from Maxwell's distribution etc.) exact and inexact differentials with their applications to thermodynamic properties. Integral calculus, basic rules for integration, integration by parts, partial fraction and substitution, Reduction formulae, applications of integral calculus.

Biology for Chemists (For Maths Students in B.Sc.)

UNIT I Cell structure and Functions **10 Hrs**

Structure of prokaryotic and eukaryotic cells, intracellular organelles and their functions, comparison of plant and animal cells. Overview of metabolic processes – catabolism and anabolism. ATP – the biological energy currency. Origin of life – unique properties of carbon, chemical evolution and rise of living systems. Introduction to biomolecules, building blocks of bio-macromolecules.

UNIT II Carbohydrate **8 Hrs**

Conformation of monosaccharides, structure and functions of important derivatives of monosaccharides like glycosides, deoxy sugars, myoinositol, amino sugars. N-acetylmuramic acid, sialic acid, disaccharides and polysaccharides. Structural polysacchrides – cellulose and chitin. Storage polysaccharides – starch and glycogen. Structure and biological functions of glycosaminoglycans or mucopolysaccharides. Carbohydrates of glycoproteins and glycolipids. Role of sugars in biological recognition. Carbohydrate metabolism. Ascorbic acid. Carbohydrate metabolism – Kreb's cycle, glycolysis, giycogenesis and glycogenolysis, gluconeogenesis, pentose phosphate pathway

UNIT III Amino-acids, Peptides and Proteins **6 Hrs**

Chemical and enzymatic hydrolysis of proteins to peptides, amino acid sequencing. Secondary structure of proteins, forces responsible for holding of secondary structures. $\alpha -$ helix, $\beta -$ sheets, super secondary structure, triple helix structure of collagen. Tertiary structure of proteinfolding and domain structure. Quaternary structure. Amino acid metabolism – degradation and biosynthesis of amino acids, sequence determination: chemical/enzymatic/mass spectral, racemization. detection.

Chemistry of oxytocin and tryptopohan releasing hormone (TRH).

UNIT IV Nucleic Acids **6 Hrs**

Purine and pyrimidine bases of nucleic acids, base pairing via H-bonding. Structure of ribonucleic acids (RNA) and deoxyribonucleic acids (DNA), double helix model DNA and forces responsible for holding it. Chemical and enzymatic hydrolysis of nucleic acids. The chemical basis for heredity, an overview of replication of DNA, transcription, translation and genetic code. Chemical synthesis of mono and trinucleoside.

PAPER-VI: MCHL-206

IInd SEM. PRACTICAL

INORGANIC CHEMISTRY PRACTICAL

1. Preparation of Coordination Compounds and their characterization by UV & IR spectra

    1- Prussian blue, turn bull's blue

    2-$[Cu(NH_3)_4]SO_4.H_2O$

    3-$K_3[Fe(C_2O_4)_3].3H_2O$

    4-$[Ni(NH_3)_6]Cl_2$

    5-Cis-$[Cr(C_2O_4)_2(H_2O)_2]$

    6-$Ni(dmg)_2$

    7-Sodium Amide

    8- Ferrocine

    9- Sodium Tetra Thionate

    10-$VO(acac)_2$

2. Gravimetric estimation of two metal ions

    (a) Cu^{2+} and Ni^{2+} (b) Cu^{2+} and Zn^{2+} (c) Ni^{2+} and Zn^{2+}

3. Iodimetric & Iodometric titrations.

ORGANIC CHEMISTRY EXPERIMENT

1. Estimation of amines /Phenol using Bromate- bromide solution or acylation method.
2. UV Spectrophotometric Estimation of

    - Amino Acids

- Proteins
- Caffeine
- Aspirin etc.

3. Extraction of organic compound from Natural sources

I- Isolation of Caffein from tea leafs

II- Isolation of Casein of lactose from milk

III- Isolation of Nicotine from tobacco

IV- Isolation of Piperine from cinchona bark

V- Isolation of Limonene from citrus fruits

PHYSICAL CHEMISTRY EXERCISE

1- Determine Enthalpy of Neutralization of strong acid and strong Base.

2- Determine Molecular weight of Binary electrolyte to find the Vant Hoff factor and degree of dissociation of electrolyte.

3- Determination of degree of dissociation of weak electrolyte 7 to study the deviation from ideal behavior that occurs with a strong electrolyte.

4- To determine the percentage composition of $CuSO_4.5H_2O$ Solution by calorimetry (Beer's law).

5- To determine partition coefficient of Benzoic Acid between water and Benzene.

6- Determination of the charge on colloidal particles.

Marks Distribution for Lab. Course for M.Sc. 2nd Semester

(a) Inorganic Chemistry Exercise: **40 Marks**

(b) Organic Chemistry Exercise: **40 Marks**

(c) Physical Chemistry Exercise: **40 Marks**

(d) Viva + Attendance +Record: **30 Marks**

(e) Seminar : **50 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 SO_2, CO_2, N_2O and C_2H_2; (b) Hydrogen Bounding 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, bio-isosterism, 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 carbyines- 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 rections, 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 Organotrasition Metal Chemistry, J. P. Collman, L. S. Hegsdus, 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 handing of reagents. Laboratory notebooks. Safety in the analytical laboratory.

(II) Errors and Evaluation **15 Hrs**

Definition of terms in mean and median. Precesion-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 analystical 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 singnificance 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 formationof 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. Sauders.
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 Eastem.
9. Basic Concepts of Analytical Chemistry, S.M. Khopkar, Wiley Easterm.
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. Ernshaw, 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, NewYork, 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 tetraoxide, 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 Heterocyc **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 cyloaddition 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 Scietific Technical.
5. Contemporary Heterocyclic Chemistry, G.R. Newkome and W.W. Paudler, Wiley-Inter Science.
6. An Introductions 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 Sciertific Publication.
10. Photochemistry, R.P. Kundall and A.Gilbert, Thomson Nelson.
11. Ornanic Photochemistry, J.Coxon and B.Halton, Chmabridge 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 compsites Nanocrystalline phase, preparation procedures, special properties, applications.

(III) Liquid Crystals **15Hrs**

Mesomorphic behaviour liquid crystals, positional order, bond orientational order, nematic and smectic mesophases; snecutenematic 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 susceptibiolity 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. Enesemble 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 fuctions, 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 unimoleular 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, McMillian.

4. Micelles, Theoretical and Applied Aspects, V. Morol, Plenum.

PAPER-VI: MCHP 309

DISSERTATION / PROJECT

Semester IV

PAPER- I: MCHC-401

SPECTROSCOPY-II **60 Hrs**

1. Mass Spectrometry **15 Hrs**

Measurement technique (El, Cl, 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). ^{1}H 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, $^{13}C^{1}H$ 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, Prenfice 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 Tends.

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.

(VI) 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, transferring, 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 – superodixide dismutase. Molybdenum oxatransferase enzymes – xanthine

oxidase. Conenzyme vitamin B_{12}.

(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 Bioinorgainc 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 Gropus **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 sythesis.

(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 hererocycles, 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.Sundbergy, 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, biosyntnesis 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. Insectcides 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 -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

Hartee-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 viscocity average molecular weights. Polydispersity and molecular weight distribution. The practical significance of molecular weight. Measurement of molecular weight. End-group, viscocity. 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 crystalling 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 Tm – 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: Caledering, die casting, rotational casting, film casting, Injection moulding, blow moulding, extrusion moulding, thermoforming, foaming, reinforcing and fibre spinning.

(V) Properties of Commerical Polymers **2 1Hrs**

Polythylene, polyvinyl chloride. Polyesters, phenolic resings, epoxy resing and silicone polymers. Functional polymers – fire retarding polymers and electrically conducting polymers. Biomedical polymers – contact lens, dental polymers, artificaial heart, kindnwy, 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 RM. Ottanbrite.
4. Contemporary Polymer Chemistry, H.R. Alcock and F.W. Lambe Prentice Hall.

Paper-VI: MHCP-409

DISSERTATION/ PROJECT