

**Nehru Gram Bharati**  
(Deemed to be university)

**KOTWA-JAMUNIPUR-DUBAWAL**  
**PRAYAGRAJ-221505**  
**UTTAR PRADESH**

**Department of Chemistry**



*Syllabus for the*

**Master of Science in chemistry**  
**(A Four Semester Course)**  
**Based on Choice based credit system**  
**(CBCS)**

**Commencing Session: 2019 – 2020**

## **Preamble of the Syllabus:**

Master of Science (M.Sc.) in Chemistry is a post-graduate course of Nehru Gram Bharati (Deemed to be University). The curriculum is prepared by following the prospectus of various national and international standards. The choice based credit system (CBCS) to be implemented through this curriculum would allow students to develop a strong footing in the fundamentals and to specialize in the disciplines of his/her liking and abilities. The students pursuing this course would have to develop in-depth understanding of various aspects of chemistry. The aim of this course is to provide conceptual understanding, development of experimental skills, designing and implementation of novel synthetic methods, developing the aptitude for academic and professional skills, acquiring the basic concepts for structural elucidation with hyphenated techniques, understanding the fundamental chemical and biological processes and rationale towards computer. The project/Dissertation introduced in the curriculum will motivate the students to pursue the research and find a job in reputed pharmaceutical and other industries in India and abroad.

### **ORDINANCE AND REGULATIONS FOR ALL POST GRADUATE - PROGRAMMES**

#### **A. ORDINANCE**

##### **1. The Degree of Master of Arts/Science/Social Science/Commerce/Law/Teacher's Education**

The Nehru Gram Bharati (Deemed to University) may confer the Degree of Mater's Programme on Such candidates who, being eligible for admission to the Post Graduate Degree Programme, have received regular instruction in the prescribed course of study, passed successfully relevant examinations and being otherwise suitable by virtue of their character, have fulfilled such other condition as may be laid down from time to time by the appropriate authorities.

##### **2. The Curriculum and Duration of Studies**

- A.** (i) The Curriculum of study of the Master Degree shall comprise of courses set out in Annexure B.  
(ii) The Departmental Committee shall prescribe the detailed content of various of study, if required before the beginning of each session. The Departmental Committee can make changes in the optional papers/subjects, subjects to the availability of teaching facility/ faculty.
- B.** The curriculum of study for the Master Degree shall be spread over four Semesters having 80 credits (each semester of 20 credits).

##### **3. Requirement for Admission**

###### **A. Registration: Registration**

- (i) Candidates of Master Degree shall first be admitted to the first semester upon the reopening of the University after summer vacation every year.

###### **(ii) Subsequent Registration**

A candidate, who fails to clear a regular course of study during any of the second, third and fourth semesters may be registered in the appropriate term of any subsequent year

to the semester concerned but within such time as enables him, to complete the study of all semester comprising Master Degree Programme within a maximum period of four years from the date of his/her registration for the first semester.

**B. Minimum Qualification For Admission**

(i) Admission to the Master Degree Programme of study shall be open to those candidates who have passed the 3 Year Graduate Degree Examination of this University or such examination of any other University or Institution after Graduation under 10+2+3 pattern as recognized by the University. Admission shall be made according to merit subject to the fulfillment of eligibility requirement as determined by the University and availability of seats in the Master courses.

**C. Conditions of Admission:**

(i) No application for registration to the First Semester shall be entertained unless it is accompanied by:

(a) A duly migration of scholastic record of the candidate, commencing from the graduation or equivalent examination.

(b) Original migration of a candidate who has been a regular student in any Institution at any time prior to making application for registration in the Faculty.

(c) Original migration certificate if the candidate is not enrolled in this University or if enrolled, his enrollment has been cancelled. Provided that if a candidate is unable to produce any of the documents other than the marks-sheet of the graduate examination at the time of seeking admission in the concerned Faculty before admission committee, he shall undertake to submit them within one month or within such further period as the University authorities may prescribe; and the admission, if any of such candidate shall until the submission of the aforesaid documents, be deemed to be provisional.

(ii) Candidate shall give also a written undertaking to the effect that:

(a) He/She shall exclusively devote his/her time to the study of courses prescribed for Master Degree and in particular he/she shall not offer any other course leading to a degree of any description whatsoever, nor shall he/she undertake any remunerative work, though with the prior permission of the Faculty, he/she may join certificate or diploma courses in any foreign language.

(b) He/She shall abide by the provision of NGB (DU) Act, Statutes, Ordinances, Regulations and Rules that are framed or may be framed there under and the orders of Officers and authorities of the University and the concerned Faculty from time to time.

**4. Fees**

The students pursuing Master Degree Programme of study shall have to pay fee as may be prescribed by the University from time to time.

5. The course of study, scheme of examination, result and promotion are covered in the regulation, and are given below.

**REGULATIONS**

1. Master Degree Programme has been divided in four semesters in two years, this is a full time course study. The odd semester would run between July to December and even semester between January to June. Two consecutive (one odd + one even) semester constitute one academic year.
2. There will be minimum 18 and maximum 24 papers /courses in all in the whole programme. Besides, there would also be one course on **Dissertation and Viva-Voce**.
3. The course has 4 components: Core courses, Elective course, Skill Development and Inter-disciplinary course.
4. Each Core course has equal weightage. Each core course will have 100 marks or 4 credits. Elective and Inter-disciplinary course will have 3 credits, whereas Skill Developments course will have 2 credits.
5. The core courses are compulsory to all students in all four semesters. The fourth (Elective course) paper and fifth (Skill Development course) paper will be opted by the students of same Department. However, the sixth (Inter-disciplinary course / University elective course) paper of each semester will be opted by the students of other Departments only.
6. In the beginning of the Semester III, the Department would announce the available specialization group/ course in the Elective Group to the students for the current session. The choice of elective group/course in the semester will be limited to those announced by the Department. Because of infrastructural and Faculty limitations, the Department may put a cap on the number of students in an elective group/course.
7. Each semester shall have minimum 90 teaching days, exclusion of holidays, admission and examinations.

### **SCHEME OF EXAMINATION**

1. The evaluation scheme of examination consists of two parts: Internal Assessment (IA), Mid Semester Exam (MSE) and End Semester Examination (ESE). Internal assessment includes Assignments, Presentations, Seminars, Quizzes, Case studies, Viva, Unit test, Group activities /Discussion, etc. The internal assessment will contribute 40% and the Semester and examination will contribute 60% to the total marks. This shall apply to both types of examination system i.e., Semester-wise and Choice based credit system (CBCS) based examination.

**\*\*Note:** The ratio of internal assessment and semester and examination will be the same as determined by the University.

2. There shall be continuous assessment of the student in each course. The course instructor shall hold a maximum of three and minimum of one internal test /assignment /presentation, etc. The distribution of marks in Internal assessment will be in two parts; 20% (Mid Sem. Exam) and 20% (Assignments/Presentations/Group Discussion etc.)

3. In case of semester examination, there shall be no binding on the number of external paper setters/examiners, though in case of CBCS//CBSS system, generally the course instructor shall be the paper setter and examiner. However, the Core courses comprising “**Dissertation and Viva-Voce** “ and “**Project Work and Viva-Voce**” respectively will be evaluated / examined by Board/s consisting of one external examiner and one internal examiner who shall be the Chairman of the Board. The Dissertation / Project Work and Viva-Voce shall equal weightage and would be judged separately. The remuneration for these courses would be at par with such courses been run in other Department of the University.
4. The duration of the End Semester Examination (ESE) of each course will be 3/2 Hours.

## M.Sc. Chemistry (Under CBCS Pattern) with effect from 2019-2020

The Course of Study and the Scheme of Examinations:

### Semester I

Sl. No.	Paper	Code	Type	Title of the paper	Credit	L+T+P	ESE.	IA	Total Marks
1.	Paper-I	CHE101	Core-1	Inorganic Chemistry-I	03	2+1+0	45	30	75
2.	Paper-II	CHE102	Core-2	Organic Chemistry-I	03	2+1+0	45	30	75
3.	Paper-III	CHE103	Core-3	Physical Chemistry-I	03	2+1+0	45	30	75
4.	Practical-I	CHEL1	Lab-1	Practical of Core Papers	03	0+0+3	45	30	75
5.	Paper-IV	CHE104-106	Elective-I		03	2+1+0	45	30	75
6.	Paper-V	CHE107	SD-1	Hand Made Soap/ Detergent Making	02	2+0+0	30	20	50
7.	Paper-VI	CHE108	UE-1	Polymer Chemistry	03	2+1+0	45	30	75
Total					20				500

### Elective Papers:

CHE104: Catalysis and Green Chemistry

CHE105: Analytical Chemistry.

CHE106: Electrochemistry.

Note: The Practical Exam shall consist of three papers (each from core papers), each of Six hr duration, suitably spread over three days and shall be at the end of Semester.

## Semester II

Sl. No.	Paper	Code	Type	Title of the paper	Credit	L+T+P	ESE.	IA	Total Marks
1.	Paper-I	CHE201	Core-4	Inorganic Chemistry-II	03	2+1+0	45	30	75
2.	Paper-II	CHE202	Core-5	Organic Chemistry-II	03	2+1+0	45	30	75
3.	Paper-III	CHE203	Core-6	Physical Chemistry-II	03	2+1+0	45	30	75
4.	Practical-II	CHEL2	Lab-2	Practical of Core Papers	03	0+0+3	45	30	75
5.	Paper-IV	CHE204-206	Elective-II		03	2+1+0	45	30	75
6.	Paper-V	CHE207	SD-2	Spectrochemical Analysis	02	2+0+0	30	20	50
7.	Paper-VI	CHE208	UE-2	Organic Chemistry (Applied Aspects Only)	03	2+1+0	45	30	75
Total					20				500

### Elective Papers:

CHE204: Nanochemistry

CHE205: Bioinorganic Chemistry.

CHE206: Bioorganic and Medicinal Chemistry.

Note: The Practical Exam shall consist of three papers (each from core papers), each of Six hr duration, suitably spread over Two/three days and shall be at the end of Semester.

### Semester III

Sl. No.	Paper	Code	Type	Title of the paper	Credit	L+T+P	ESE.	IA	Total Marks
1.	Paper-I	CHE301	Core-7	Specialization Paper-I (A/I/O/P)*	03	2+1+0	45	30	75
2.	Paper-II	CHE302	Core-8	Specialization Paper-II (A/I/O/P)*	03	2+1+0	45	30	75
3.	Paper-III	CHE303	Core-9	Specialization Paper-III (A/I/O/P)*	03	2+1+0	45	30	75
4.	Practical-III	CHEL3	Lab-3	Practical (A/I/O/P)*	03	0+0+3	45	30	75
5.	Paper-IV	CHE304-306	Elective-III		03	2+1+0	45	30	75
6.	Paper-V	CHE307	SD-3	Industry Visit (7-15 Days)	02	2+0+0	30	20	50
7.	Paper-VI	CHE308	UE-3	Environmental Chemistry	03	2+1+0	45	30	75
Total					20				500

\*The choice of Specialization in the semester will be subjected to the infrastructural and Faculty limitations

#### **Elective Papers:**

CHE304: Organometallic Chemistry of Transition Metals

CHE305: Forensic Analysis

CHE306: Concepts in Organic Synthesis

Note: The Practical Exam in each specialization shall consist of three papers (each from core papers), each of Six hr duration, suitably spread over two/three days and shall be at the end of Semester.



## Semester IV

Sl. No.	Paper	Code	Type	Title of the paper	Credit	L+T+P	ESE.	IA	Total Marks
1.	Paper-I	CHE401	Core-4	Specialization Paper-IV (A/I/O/P)*	03	2+1+0	45	30	75
2.	Paper-II	CHE402	Core-5	Specialization Paper-V (A/I/O/P)*	03	2+1+0	45	30	75
3.	Paper-III	CHE403	Core-6	Specialization Paper-VI (A/I/O/P)*	03	2+1+0	45	30	75
4.	Project Work	CHEL4	Project/ Dissertation		03	0+0+3	45	30	75
5.	Paper-IV	CHE404-406	Elective-II		03	2+1+0	45	30	75
6.	Paper-V	CHE407	SD-2	Computer Application in Chemistry	02	2+0+0	30	20	50
7.	Paper-VI	CHE408	UE-2	Nano-chemistry	03	2+1+0	45	30	75
Total					20				500

### Elective Papers:

CHE404: Physical Methods in Chemistry

CHE405: Principle and Applications of Luminoscence Spectroscopy

CHE406: Advances in Nucleic Acid and Lipid Chemistry

Note: The Practical Exam in each specialization shall consist of three papers (each from core papers), each of Six hr duration, suitably spread over two/three days and shall be at the end of Semester.

### Project/Dissertation (CHE-L4)

Individual faculty members will float stipulated number of projects at the end of III SEM. Students have to consult respective faculty members and select projects. More than one student can work under a single project based on nature of the project. Guide allotment for MSc project will be based on choice cum merit.

Once guide allotment (either single or more than one guide) is declared, student has to submit research proposal and give a presentation, either individually or one member from the group. Research proposal and presentation carries 10 marks. Students will be periodically assessed for their project work by individual faculty member or group of faculty members. The final submission of the research project, i.e., small thesis, presentation and comprehensive viva carries 35 marks.

Note:

1. Student should submit 3 copies of the final research project copy in hard binding format with all declarations and signatures.
2. For referencing any ACS journal pattern should be followed.

### SCHEME OF EXAMINATIONS

1. English shall be the medium of the instruction and examination.

2. Examination shall be conducted at end of each semester as per the academic calendar notified by the Nehru Gram Bharti (Deemed to be University).
3. The system of evaluation shall be as follows:
  - 3.1. Each course will carry 25 marks for every credit, of which 40% shall be reserved for internal assessment based on classroom participation, seminar, term courses, testes and attendance. The weightage given to each of these components shall be decided and announced at the beginning of the semester by the individual teacher responsible for the course. Any student who fails to participate in classes, seminars, term courses, tests, will have to face disciplinary action decided by the university.
  - 3.2. The remaining 60% marks in each paper shall be awarded on the basis of a written examination at the end of each semester. The duration of written examination for each paper shall be three hours and the practical examination shall be of six hours. The paper of written examination shall be divided in to two sections and a candidate has to answer 5 questions of equal marks.
  - 3.3. A candidate is allowed to reappear **ONLY** in **THEORY** papers to improve his/her previous performance.
4. Examinations for courses shall be conducted only in the respective odd and even semesters as per the Scheme of Examinations. Regular as well as Ex-Students shall be permitted to appear/re-appear/improve in courses of Odd Semesters only at the end of Odd Semesters and courses of Even Semesters only at the end of Even Semesters.

**Syllabus**  
M.Sc (Chemistry)

*Semester I*

**Inorganic Chemistry I (CHE-101)**

**Unit I**

Review of Bohr's theory, its limitations and atomic spectrum of hydrogen atom. Wave mechanics: de Broglie equation, Heisenberg's Uncertainty Principle and its significance. Schrödinger's wave equation, significance of  $\psi$  and  $\psi^2$ . Quantum numbers and their significance. Normalized and orthogonal wave functions. Sign of wave functions. Radial and angular wave functions for hydrogen atom. Radial and angular distribution curves. Shapes of s, p, d and f orbitals. Pauli's Exclusion Principle, Hund's rule of maximum multiplicity, aufbau principle and its limitations.

**Unit II**

Bonding and structure: Types of bonds, orbital symmetry and overlaps, concept of MO and VB theory, concept of hybridization, bond energy and covalent radii, concept of resonance, molecular dipole moment; polarizing power and polarizability, Fajan's rules.

**Unit III**

Inorganic Spectroscopy I: Number of microstates and term symbols for gaseous free atoms and ions. Spin-orbit coupling in free ion terms. Hund's rules. Splitting of spectroscopic terms of  $p^2$  and  $d^2$  configurations.

**Unit IV**

Inorganic Spectroscopy II: Principles of Electronic Spectroscopy-Franck-Condon principle, selection rules, band intensities and vibronic coupling Band width. Different types of electronic transitions and molar absorption coefficient.

**Unit V**

Introduction to transition metal complexes: Brief review of the general characteristics of transition elements, types of ligands, nomenclature of coordination complexes, chelates, chelate effect, geometry and isomerism, formation of complexes, stability constants, Werner, Sidzwick and VSEPR theory.

**Books Suggested** (Names of Publishers may vary as per copyright status):

1. Principles of Inorganic Chemistry, B.R.Puri, L.R. Sharma, K.C. Kalia, Milestone Publishers and Distributors/ Vishal Publishing Co.
2. Advanced Inorganic Chemistry, F.A. Cotton and Wilkinson, John Wiley.
3. Concise Inorganic Chemistry, J.D. Lee, Wiley.
4. Inorganic Chemistry, J.E. Huhey, Harpes& Row.
5. Chemistry of the Elements. N.N. Greenwood, A. Earnshaw, Pergamon.
6. Inorganic Electronic Spectroscopy, A.B.P. Lever, Elsevier.
7. Comprehensive Coordination Chemistry eds., G. Wilkinson, R.D. Gillars and J.A. Mc Cleverty, Pergamon.

**Organic Chemistry I (CHE-102)**

**Unit I**

Principles of stereochemistry: Configurational and conformational isomerism in acyclic and cyclic compounds; stereogenicity, stereoselectivity, enantioselectivity, diastereoselectivity and asymmetric induction.

**Unit II**

Aromaticity: Benzenoid and non-benzenoid compounds – generation and reactions.

**Unit III**

Organic reactive intermediates; Generation, stability and reactivity of carbocations, carbanions, free radicals, carbenes, benzyne and nitrenes.

**Unit IV**

Aliphatic Nucleophilic Substitution:

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

The neighbouring group mechanism, neighbouring group participation by p and s bonds, anchimeric assistance. Classical and nonclassical carbocations, phenonium ions, norbornyl system, common carbocation rearrangement. The  $S_Ni$  mechanism. Nucleophilic substitution at an allylic, aliphatic trigonal and vinylic carbon. Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium, phase transfer catalysis, ambient nucleophile and regioselectivity.

**Unit V**

Conformational Analysis:

Stability factors for conformation: Torsional strain, Vander Waal's interaction, Hyperconjugation, dipole-dipole interaction, hydrogen bonding and anomeric effect.

Conformation of n-butane, ethane-1,2-diol, 1,2-difluoroethane.

Conformational analysis of substituted cyclohexane: 1,2-dimethyl cyclohexane, Dihydroxy cyclohexane, t-butyl cyclohexene, conformational analysis of cyclohexene, conformational analysis of decaline.

**Books Suggested**(Names of Publishers may vary as per copyright status):

1. Advanced Organic Chemistry, Jagdamba Singh, PragatiPrakashan.
2. Organic Chemistry: Concepts and Applications, Jagdamba Singh, PragatiPrakashan.
3. Advanced Organic Chemistry-Reactions, Mechanism and Structure, Jerry March, John Wiley.
4. Advanced Organic Chemistry Part A: Structure and Mechanisms, Francis A. Carey, Richard J. Sundberg, Springer.
5. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.
6. Structure and Mechanism in Organic Chemistry, C.K. Ingold, Cornell University Press.
7. Organic Chemistry, R.T. Morrison, R.N. Boyd, Prentice-Hall.
8. Reaction Mechanism in Organic Chemistry, S.M. Mukherji, S.P. Singh, Macmillan.
9. Stereochemistry of Organic Compounds, D. Nasipuri, New Age International.
10. Stereochemistry of Organic Compounds, P.S. Kalsi, New Age International.

### **Physical Chemistry I (CHE-103)**

#### **Unit I**

Origin of quantum theory. Black body radiation. Wien and Rayleigh Jeans laws. Planck's law and energy of harmonic oscillator.

#### **Unit II**

Concept of operators in quantum mechanics- operators for velocity, kinetic energy, momentum and angular momentum. Laplacian and Hamiltonian operator, Schrödinger's equation and its solution for Hydrogen atoms. Derivation of Heisenberg's uncertainty principle.

#### **Unit III**

Quantum mechanical approaches to molecular Bonding, Born-Oppenheimer approximation. Valence bond theory and molecular orbital theories. Valence bond theory and its application to homonuclear (Hydrogen) and heteronuclear (HCl) diatomics.

#### **Unit IV**

LCAO-MO treatment of hydrogen molecule ion. Comparative study of MO and VB theory. The variation theorem, linear variation principle. Perturbation theory (First order and nondegenerate). Applications of variation method and perturbation theory to the Helium atom.

### **Unit V**

Huckel molecular orbital theory and its application to hybridization systems (ethylene, butadiene, allyls and benzene). Calculation of delocalization energy. Physical significance of charge density and bond order. Calculation of bond length. Perturbation methods in LCAO-MO theory. Extended Huckel molecular orbital theory and SCF-MO method.

**Books Suggested**(Names of Publishers may vary as per copyright status):

1. Introduction to Quantum Chemistry, A.K. Chandra, Tata Mc Graw Hill.
2. Quantum Chemistry, Ira N. Levine, Prentice Hall.
3. Introduction to Quantum Chemistry-R.K. Prasad, New Age Publication.
4. Physical Chemistry, P.W. Atkins, ELBS.
5. Physical Chemistry, Levine
6. Chemical Kinetics. K.J. Laidler, McGraw-Hill.
7. Physical Chemistry, G. W.Castellan.

### **Chemistry Laboratory (CHE-L1)**

#### **Inorganic Chemistry:**

1. Qualitative analysis of inorganic mixture for seven radicals only (including interfering radicals, insolubles, and two rare elements).
2. Quantitative separation and estimation of individual metal component from binary mixture solution (either both component gravimetrically or one component gravimetrically and other one volumetrically).

#### **Organic Chemistry:**

Organic synthesis: Any two from

Acylation: Acetylation of cholesterol and separation of cholesteryl acetate by column chromatography.

Oxidation: Adipic acid by chromic acid oxidation of cyclohexanol.

Aldol condensation: Dibenzalacetone from benzaldehyde.

Sandmeyer reaction: p-Chlorotoluene from p-toluidine.

Cannizzaro reaction: p-Chlorobenzaldehyde as substrate.

Friedel Crafts reaction: Benzoyl propionic acid from succinic anhydride and benzene.

Aromatic electrophilic substitutions: Synthesis of p-bromoaniline.

Rearrangement: Synthesis of benzilic acid by benzil-benzilic acid rearrangement. Pinacol-pinacolone rearrangement in Benzpinacol.

### **Physical Chemistry:**

1. Determine the concentration or percentage of one or two optically active substances in the given solution polarimetrically.
2. Kinetics of oxidation of reducing sugars by potassium ferricyanide/copper(II) in presence of ammonium hydroxide or sodium hydroxide.
3. Kinetics of oxidation of alcohols/diols by aqueous alkaline hexacyanoferrate (III) ions.
4. Potentiometric titration of weak/strong acid and strong /weak base.

### **Elective Papers:**

#### **Catalysis and Green Chemistry (CHE-104)**

##### Unit I

Basic Principles of Green Chemistry: Prevention of waste by products, maximum incorporation of the reactants into the final product, prevention or minimization of hazardous products, designing safer chemicals, energy requirements for synthesis, selection of appropriate solvent, selection of starting materials, use of protecting groups.

##### Unit II

Green Reagent: Dimethylcarbonate, polymer supported reagent, polymer supported peracids, Poly-N-bromosuccinimide (PNBS), sulfonazide polymer, polystyrene Wittig reagent and polymer supported peptide coupling agent, miscellaneous reagents.

##### Unit III

Introduction and Basic concept of green catalysis, Application of catalyst functionality, concepts for control of reaction, selectivity and kinetic models. Steps in catalytic reaction (Adsorption and Kinetic models). Selection and design and Preparation of catalysts.

## Unit IV

Green Catalyst: Acid catalyst, oxidation catalyst, basic catalyst, polymer supported catalyst, polystyrene – aluminium chloride, polymer supported photosensitizers, miscellaneous illustration and solid support reagents.

## Unit V

Aqueous Phase Reactions: Diels-Alder reaction, Claisen rearrangement, Wittig-Horner reaction, Michael reaction, Aldol condensation, Knoevenagel reaction, Pinacol coupling, Benzoin condensation, Claisen- Schmidt condensation. Strecker synthesis, Wurtz reaction, Oxidations, Reductions, Polymerization reactions, photochemical reactions, electrochemical synthesis & miscellaneous reactions in Aqueous Phase.

Books Suggested(Names of Publishers may vary as per copyright status):

1. New Trends in Green Chemistry, V.K. Ahluwalia, M.Kidwai, Anamaya publishers, New Delhi.
2. Introduction to Green Chemistry, V.Kumar.
3. Green Chemistry: Theory and Practice, Paul T. Anasta, John C. Warner, Oxford University Press.
4. Catalysis: Concepts and Green Applications, Gadi Rothenberg, Wiley.

## **Analytical Chemistry (CHE-105)**

### Unit I

Introduction to Analytical Chemistry- Methods of qualitative and quantitative analysis.

### Unit II

Thermal Analysis: Introduction, types and applications of thermoanalytical methods, thermogravimetry etc.

### Unit III

Electro Analytical Techniques: Voltametry, Amperometry, Coulometry, Conductometry, Potentiometry.

### Unit IV

Diffraction Techniques: Introduction, types and applications with special reference to x-ray diffraction technique.

### Unit V

Electrochemical Techniques: Introduction and applications of Electrolysis, Electrophoresis.



**Books Suggested**(Names of Publishers may vary as per copyright status):

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

**Electrochemistry (CHE-106)**

Unit I

Equilibrium electrochemistry: Activities in electrolytic solutions, mean activity coefficient, Debye-Huckel treatment of dilute electrolyte solutions, origin of electrode potential, half-cell potential, electrochemical cell, Nernst equation, thermodynamics of electrochemical cell.

Unit II

Dynamic electrochemistry: Electrical double layer - electrode kinetics, rate of charge transfer, current density, Butler- Volmer equation,

Unit III

Introduction to polarography, cyclic voltammetry, theory of corrosion and inhibition of corrosion.

Unit IV

Bioelectrochemistry: bioelectrodics, membrane potentials, simplistic theory, modern theory, electrical conductance in biological organism: electronic, protonic electrochemical mechanism of nervous systems, enzymes as electrodes.

Unit V

Electrochemical sensors: Potentiometric sensors, Ion-selective electrodes, Membrane electrodes, Amperometric sensors, Clark and Enzyme electrodes).

**Books Suggested**(Names of Publishers may vary as per copyright status):

1. Modern Electrochemistry, Vol. 1, Vol. 2A and Vol. 2 B, J.O'M. Bockris, A.K.N. Reddy, Plenum Press, New York.
2. Electrochemical Methods: Fundamentals and Applications, A.J. Bard, L.R. Faulkner, John Wiley and Sons, New York.

## Skill Development Paper

### Hand Made Soap/Detergent Making (CHE-107)

1. Theory of Soap/Detergent :
2. Types of cleaning agents: (1) Toilet Soaps (2) Washing Soap (3) Detergent Powder - High and Medium quality (4) Dish Wash Powder (5) Cleaning Lotion (6) Liquid Soap.
3. Properties of cleaning agents
4. Technical skill of soap/detergent making
5. Marketing of soap and allied products

## University Elective Paper

### Polymer Chemistry (CHE-108)

1. Introduction: Classification of polymers, intermolecular forces in polymers.
2. Mechanism and kinetics of step-growth and chain growth polymerization: Radical, cationic, anionic and condensation polymerization, copolymerization, reactivity ratios, thermodynamic aspects of polymerization, mechanism of living radical polymerizations: nitroxide mediated polymerization (NMP), metal-catalyzed living radical polymerization, reversible addition-Fragmentation Chain Transfer (RAFT) radical polymerization, coordination polymerization, ring opening polymerization, click chemistry.
3. Polymer solutions: Flory-Huggins theory of polymer solutions, nature, size and shape of macromolecules in solution.
4. Polymer structure and Physical properties: Microstructure of polymer chains, crystallinity in polymers, glass transition temperature, rheological properties, molecular weight and its distribution.
5. Specialty polymers: Liquid crystalline polymers, conducting polymers, electroluminescent polymers, inorganic polymer, nanocomposites of polymers, biomedical polymers.

### Books Recommended

1. Text Book of Polymer Science, 3<sup>rd</sup> Edition (1984), F. W. Billmayer, Jr., Willey-Interscience, New York.
2. Physical Chemistry, 8<sup>th</sup> Edition, P. W. Atkins, Oxford University Press, New York. **YEAR**
3. Principles of Polymerization, 3<sup>rd</sup> Edition (1991) G. Odian, John Wiley, Singapore
4. Principle of Polymer Sciences, P. Bahadur and N.V. Sastry, Narosa Publishing House, New Delhi (2002)
5. Polymer Sciences, V.R. Gowariker, N.V. Vishwanathan, J. Shreedhar , Wiley Eastern, New Delhi (1986)

## *Semester II*

### **Inorganic Chemistry II (CHE-201)**

#### **Unit I**

Theories of the co-ordinate linkage: Valence bond, crystal field, ligand field and molecular orbital theories. Crystal field splitting of d-orbitals in octahedral, trigonal bipyramidal, square pyramidal, tetragonal and square planar fields. Crystal field stabilization energy (CFSE). M.O. energy level diagram for octahedral and tetrahedral complexes (with s bonding only). Spectrochemical series.

#### **Unit II**

Electronic absorption spectra of transition metal complexes. Orgel diagrams for  $d^1$ ,  $d^4$ ,  $d^6$  and  $d^9$  configurations with D ground state. Jahn-Teller effect. Stabilization of less familiar oxidation states of transition metals via coordination.

#### **Unit III**

Metal Carbonyls and Nitrosyls: Mononuclear and polynuclear carbonyls and their structures. Nature of M-C-O bonding. Preparation of metal carbonyls and their reactions. Metal nitrosyls-bonding and structure. Metal carbonyl-nitrosyl complexes.

#### **Unit IV**

Chemistry of f-Block Elements: Comparative study of lanthanides and actinides with special reference to electronic structure. Oxidation state, coordination number, structure, stereochemistry and magnetic and spectral properties.

#### **Unit V**

General chemistry of actinides including E.M.F. diagrams. Extraction and metallurgy of thorium and uranium. Technical production of plutonium. Separation of transamericium elements.

**Books Suggested**(Names of Publishers may vary as per copyright status):

1. Advanced Inorganic Chemistry, F.A. Cotton, Wilkinson, John Wiley.
2. Inorganic Chemistry: Principles of Structure and Reactivity, Huheey, Medhi, Pearson Education India.
3. Physical Methods in Inorganic Chemistry, R S.Drago, Affiliated East-West Press Pvt. Ltd.
4. Chemistry of the Elements. N.N. Greenwood, A. Earnshaw, Pergamon.
5. Inorganic Electronic Spectroscopy, A.B.P. Lever, Elsevier.

6. Comprehensive Coordination Chemistry eds., G. Wilkinson, R.D. Gillars, J.A. McCleverty, Pergamon.

## **Organic Chemistry II (CHE-202)**

### **Unit I**

Electrocyclic and cycloaddition reactions:

Cycloadditions-antifacial and suprafacial additions,  $4n$  and  $4n+2$  systems,  $2+2$  addition of ketenes, 1,3-dipolar cycloadditions and cheletropic reactions

### **Unit II**

Pericyclic Reaction:

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.

Suprafacial and antarafacial shift of H, sigmatropic shifts involving carbon moieties, retention and inversion of configuration, (3,3) and (5,5) sigmatropic rearrangements, detailed treatment of Claisen and Cope-rearrangements. Fluxional tautomerism, Aza-Cope rearrangements. Introduction to Ene reactions. Simple problems on pericyclic reactions.

### **Unit III**

Aromatic Nucleophilic Substitution:

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

### **Unit IV**

Addition to Carbon-Hetero Multiple Bonds:

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, Mannich, Benzoin, Perkin and Stobbe reactions. Hydrolysis of esters and amides, ammonolysis of esters.

## **Unit V**

Elimination Reactions:

The E<sub>2</sub>, E<sub>1</sub> and E<sub>1cB</sub> 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.

**Books Suggested**(Names of Publishers may vary as per copyright status):

1. Advanced Organic Chemistry, Jagdamba Singh, PragatiPrakashan.
2. Organic Chemistry: Concepts and Applications, Jagdamba Singh, PragatiPrakashan.
3. Advanced Organic Chemistry Part A: Structure and Mechanisms, Francis A. Carey, Richard J. Sundberg, Springer.
4. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.
5. Structure and Mechanism in Organic Chemistry, C.K. Ingold, Cornell University Press.
6. Organic Chemistry, R.T. Morrison, R.N. Boyd, Prentice-Hall.
7. Reaction Mechanism in Organic Chemistry, S.M. Mukherji, S.P. Singh, Macmillan.

## **Physical Chemistry II (CHE-203)**

### **Unit I**

Quantum states and complexions. The combinatory rule. System with definite total energy. Degeneracy of energy levels Probability and most probable distribution. Indistinguishability. Maxwell-Boltzmann statistics, partition function. Translational, rotational, vibrational and electronic partition functions. Internal energy and heat capacity in terms of partition function.

### **Unit II**

Indistinguishability of gas molecules. Maxwell-Boltzmann law for gaseous system. Thermodynamic functions for gaseous systems. Molar heat capacity of gases. Heat capacity of hydrogen at low temperatures. Heat capacities of monatomic crystals. The Einstein model. Debye's theory of solid. Heat capacities of crystals at very low temperatures. Calorimetric entropy. Spectroscopic entropy, Comparison of calorimetric and spectroscopic entropies.

### **Unit III**

Third Law of thermodynamics (i) Nernst heat theorem, (ii) Entropy of chemical reactions (iii) statements of third law of thermodynamics and (iv) Conventional entropies.

## Unit IV

Expression for equilibrium constant in terms of partition functions. Equilibrium constants of simple systems - (i) Ionization of metal atoms, (ii) Dissociation of diatomic molecules and (iii) Isotopic exchange equilibria. Calculation of thermodynamic properties from spectroscopic data.

## Unit V

Bose- Einstein statistics, Fermi-Dirac Statistics, Comparison of M-B, B-E and F-D statistics. Fermi-Dirac gas (electron gas in metals), Bose-Einstein gas (liquid Helium).

**Books Suggested**(Names of Publishers may vary as per copyright status):

1. Physical Chemistry, P.W. Atkins, ELBS.
2. Physical Chemistry, Levine
3. Thermodynamics, Gurdeep Raj
4. Chemical Kinetics. K.J. Laidler, McGraw-Hill.
5. Physical Chemistry, G. W.Castellan.
6. Kinetics and Mechanism of Chemical Transformation J.Rajaraman, J.Kuriacose, Mc Millan.
7. Introduction to Polymer Science, V.R. Gowarikar, N.V. Vishwanathan, J.Sridhar, Wiley Eastern.
8. Polymer Chemistry, B. K. Sharma.

## Chemistry Laboratory (CHE-L2)

### Inorganic Chemistry:

Preparation of Coordination Complexes and their Characterization by m.p, elemental Analysis and molar conductivity measurements (Any two).

- (a)  $\text{VO}(\text{acac})_2$
- (b)  $\text{K}_3[\text{Cr}(\text{C}_2\text{O}_4)_3] \cdot 3\text{H}_2\text{O}$
- (c)  $\text{Na}[\text{Cr}(\text{NH}_3)_2(\text{SCN})_4]$
- (d)  $\text{Mn}(\text{acac})_3$
- (e)  $\text{K}_3[\text{Fe}(\text{C}_2\text{O}_4)_3]$
- (f)  $\text{Hg}[\text{Co}(\text{SCN})_4]$
- (g)  $[\text{Co}(\text{Py})_2\text{Cl}_2]$
- (h)  $[\text{Ni}(\text{NH}_3)_6]\text{Cl}_2$

Study of recorded UV-visible and IR of above prepared coordination compounds.

### Organic Chemistry:

- (a) Preparation of various organic compounds involving two or three steps employing different reactions viz. Aldol Condensation, reactions of enolate ions, oxidation reactions,

Cannizzarro reaction, Molecular rearrangement reactions etc. with a view to give the student sufficient synthetic training in synthetic organic chemistry

(b) Isolation of:

a. Caffeine from tea leaves

b. Eugenol from cloves

**Physical Chemistry:** (Any two exercise)

(i) Determination of the velocity constant of the reaction between acetone and iodine catalysed by HCl/H<sub>2</sub>SO<sub>4</sub>.

(ii) Determination of velocity constant of saponification of ethyl acetate with sodium hydroxide.

(iii) Kinetics of reaction between copper sulphate and sugars in alkaline medium.

(iv) Titration of acid versus base using pH meter and calculation of pK<sub>a</sub> value of an acid.

(v) Elevation of boiling point using Landberger's apparatus.

(vi) To study the adsorption of oxalic acid on activated charcoal and test the validity of Freundlich's adsorption isotherm.

(vii) Rast method for determining molar mass.

## **Elective Papers**

### **Nanochemistry (CHE-204)**

#### Unit I

Introduction: History scope and perspectives of nanochemistry. Synthesis and Stabilization of Nanoparticles, Chemical Reduction; Reactions in Micelles, Emulsions, and Dendrimers; Photochemical and Radiation Chemical Reduction.

#### Unit II

Experimental Techniques: Transmission and scanning electron microscopy, Probe Microscopy, X-ray diffraction, Neutron diffraction, Miscellaneous Techniques, Comparison of Spectral Techniques used for Elemental Analysis.

#### Unit III

Size Effects in Nanochemistry: Models of Reactions of Metal Atoms in Matrices; Properties; Kinetic Peculiarities of Chemical Processes on the surface of Nanoparticles; Thermodynamic Features of Nanoparticles.

#### Unit IV

Applications of Nanoparticle in various fundamental research, industries, medical field.

#### Unit V

Environmental issue; toxicity, biosafety and ethical issue in applications of Nanoparticle.

**Books Suggested** (Names of Publishers may vary as per copyright status):

1. Nanomaterials and Nanochemistry, edited by C. Brechignac, P. Houdy, M. Lahmani, Springer-Verlag, Berlin.
2. Nanoparticle Technology Handbook. M. Hosokawa, K. Nogi, M. Naito, T.Yokoyama (Eds.), Elsevier.
3. Nanotechnology Basic Calculations for Engineers and Scientists, Louis Theodore, John Wiley and Sons.
4. Nanochemistry: A Chemical Approach to Nanomaterials, Geoffrey A Ozin, André Arsenault, Ludovico Cademartiri, RSC Publishing.

### **Bioinorganic Chemistry (CHE-205)**

#### Unit I

Complexes of Biological Significance: Metal complexes of amino acids and peptides. Metal complexes of nucleic acid bases, nucleosides and nucleotides. Metal complexes of porphyrins and pthalocyanins.

#### Unit II

Synthetic model oxygen carrier complexes and model dinitrogen complexes. Phosphates and bioenergetics. Phosphorylation and phosphorolysis. Adenine nucleotides in metabolic energy transfer. Oxidation of glucose and the role of phosphate.

#### Unit III

Role of Metal Ions in Biological Systems: Essential and trace metal ions. Metal ions storage and transport (Na, K, Ca, Mg, Fe, Cu and Zn)-Ferritin and Transferrin. Metal ion toxicity and its cure by chelating agents. Pharmacological activity and metal chelates. Carcinogenic metals, carcinogenic and carcinostatic ligands.

#### Unit IV

Metallo Proteins and Metallo Enzymes: Function, electronic structure, bonding and stereochemistry of the active site. Natural Oxygen Carrying Proteins-Haemoglobin, Myoglobin, Hemerythrins and Hemocyanin,

#### Unit V

Electron Transport Proteins (a) Iron-Sulfur Proteins-Rubredoxin and Ferredoxins, (b) Cytochromes (types a, b and c).

**Books Suggested** (Names of Publishers may vary as per copyright status):



1. Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, An Introduction and Guide, W. Kaim, B. Schwederski, Wiley, New York.
2. Inorganic Chemistry of Biological Processes, M. N. Hughes, John-Wiley and Sons, New York.
3. Principles of Bioinorganic Chemistry, S. J. Lippard, J. M. Berg, University Science Books.
4. Bioinorganic Chemistry, I. Bertini, H. B. Grey, S. J. Lippard, J. S. Valentine, Viva Books Pvt. Ltd., New Delhi.

## **Bioorganic and Medicinal Chemistry (CHE-206)**

### Unit I

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

### Unit II

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

### Unit III

Relationship of chemical structure and biological activities and theories of drug action. Detailed study of following classes:

(i) Antineoplastic Agents: Introduction, cancer chemotherapy, role of alkylating agents and antimetabolites in treatment of cancer. Mention of carcinolytic antibiotics and mitotic inhibitors. Synthesis of mechlorethamine, cyclophosphamide, melphalan, uracil, amustards, and 6-mercaptopurine products.

(ii) Cardiovascular Drugs: Cardiovascular diseases, drug inhibition of peripheral sympathetic function. Direct acting arteriolar dilators. Synthesis of amyl nitrate, hydralazine, verapamil, methyl dopa and diazoxide propanol.

### Unit IV

(i) Local Anti-infective Drugs: Antitubercular drugs and Antimalarial drugs: Introduction and general mode of action. Study of sulphonamides, ciprofloxacin, norfloxacin, amino salicylic acid.

(ii) Psychoactive Drugs: CNS depressants general anaesthetics, hypnotics, sedatives, anti-anxiety drugs, benzodiazepines. Antipsychotic drugs: diazepam, alprazolam, trimethadione, barbiturates and glutethimide.

(iii) Antibiotics: Penicillin G, chloramphenicol, cephalosporin, tetracycline and streptomycin.

#### Unit V

Vitamins and Hormones: Detailed study of chemistry of Vit. B1, Vit. C1, Pantothenic acid, Biotin (Vitamin H) and  $\alpha$ -tocopherol (Vitamin E). Biological action of vitamins.

Insect hormones : Pheromones and Juvenile hormones; Plant hormones: Gibberellins.

Books Suggested(Names of Publishers may vary as per copyright status):

1. Introduction to Bioorganic Chemistry and Chemical Biology, David Van Vranken, Gregory A, Garland Science (Taylor & Francis).
2. Natural Products Chemistry, Jagdamba Singh, PragatiPrakashan.
3. Chemistry of Natural Products, R.H. Thomson, Wiley, New York.
4. Organic Chemistry, Volume 2: Stereochemistry and the Chemistry Natural Products, I.L.Finar, Pearson Education India.

## Skill Development Paper

### Spectrochemical Analysis (CHE-207)

1. **Nuclear Magnetic Resonance Spectroscopy:** Theory of nuclear magnetic resonance, Applications of  $^1\text{H}$  NMR,  $^{13}\text{C}$ ,  $^{31}\text{P}$  NMR, Quantitative applications of NMR: Drug Analysis, Molecular Weight determination.
2. **Electron Spin Resonance Spectroscopy:** Theory, Instrumentation and Important analytical applications
3. **Electron Spectroscopy:** Theory, Instrumentation and applications of Electron spectroscopy (XPS, XRF and Auger),
4. **Plasma Emission Spectroscopy:** Theory. Instrumentation and Analytical applications of inductively coupled plasma emission spectroscopy (ICPE).
5. **Applications in analysis of special materials:** Analysis of dairy products and petrochemicals

#### Books Recommended

1. D.A. Skoog, F.J. Holler and T.A. Nieman, *Principles of Instrumental Analysis*, 5<sup>th</sup> Edition (1998), Harcourt Brace & Company, Florida.
2. R.L. Pecsok, L. D. Shields, T. Cairns and L.C. Mc William, *Modern Methods of Chemical Analysis*, 2<sup>nd</sup> Edition (1976), John Wiley, New York.
3. J.M. Hollas, *Modern Spectroscopy*, 3<sup>rd</sup> Edition (1996), John Wiley, New York.
4. H.A. Strobel, *Chemical Instrumentation – A Systematic Approach*, 2<sup>nd</sup> Edition (1973), Addison Wesley, Mass.
5. D.C. Garratt, *the Quantitative Analysis of Drugs*, 2<sup>nd</sup> Edition (1992), Chapman and Hall Ltd., London.
6. W. Horwitz (Editor), *Official Methods of Analysis*, 11<sup>th</sup> Edition (1970), Association of Official Analytical Chemists, Washington DC.

## University Elective Paper

### Organic Chemistry (Applied Aspects Only) (CHE-208)

#### 1. Organic chemistry and industry

2. **Life begins with nucleic acids.** Sugar alcohols, *S*-glycosides. vitamin-C and inositols
3. **Brief introduction of the following with context to life:** Aspirin, adrenaline, coniine, thujone, cholesterol, prostaglandins, penicillines.
4. **Crixivan**-organic Chemists' answer to HIV.
5. **Bio-polymers:** polysaccharides - starch, cellulose, sucrose, amino acids and polypeptides, proteins.
6. **Synthetic polymers:** properties and uses - Polyester, poly-tetrafluoroethylene, polyamino acids, polycyanoacrylates, polyurethanes, silicone rubbers, polymeric antioxidants, polyphosphazenes, divinylether - maleic anhydride cyclopolymer (DIVEMA)

#### Books Recommended

1. Yescombe, Sources of information on rubber, plastic and allied industries, Pergamon Press, 1968.
2. Peter Bernfeld, Biogenesis of Natural compounds, 2nd edition, Pergamon press, 1967.
3. J. Clayden, N. Greeves, S. Warren and P. Wothers, Organic chemistry, Oxford University press INC, New York, 2001
4. Harry R. Allcock, Frederick W. Lampe and James E. Mark, Contemporary Polymer Chemistry, 3<sup>rd</sup> edition, Pearson Prentice Hall, 2005

## *Semester III*

\*For core papers of Specializations please see at the end of the syllabus

### **Elective Paper**

#### **Organometallic Chemistry of Transition Metals (CHE-304)**

##### Unit 1

Inorganic  $\pi$  Acid Ligands: Dioxygen and dinitrogen, nitrosyl, tertiary phosphines and arsines as ligands. Complexes of  $\sigma$  donor ligands: Transition metal alkenyls, alkynyls, carbenes and carbinos.

##### Unit II

$\pi$  complexes of unsaturated molecules: Preparation, bonding and structure of alkene, alkyne, allyl, dienyl and trienyl complexes; reactions with special reference to organic synthesis.

##### Unit III

Transition organometallic compounds:

Transition metal compounds with bonds to hydrogen, boron, silicon

##### Unit IV

Transition metal compounds in catalysis: Hydrogenation, hydroformylation and polymerization; Wacker Process.

##### Unit V

Transition metal Compounds with M-H bonds: Metal hydrides (classical and non classical). Agostic interaction. Application of NMR in studying hydrido complexes.

**Books Suggested** (Names of Publishers may vary as per copyright status):

1. Advanced Inorganic Chemistry, F.A. Cotton, G. Wilkinson, John Wiley and Sons, NY.
2. The Organometallic Chemistry of Transition Metals, R. H. Crabtree, John Wiley.
3. Principles and Applications of Organotransition Metal Chemistry, J.P. Collman, L.S. Hegedus, J.R. Norton, R.G. Finke, Univ. Sci. Books, Mill Valley. California.

#### **Forensic Analysis (CHE-305)**

##### Unit I

Introduction: Profile of a forensic laboratory, Forensic Scientists' role and quality control, Crime-scene investigation, Collection and preserving physical evidences and evidentiary documentation, Future prospects of forensic analysis

## Unit II

Real Case Analysis: Liquor analysis, Trap-case analysis, Petroleum product analysis, Fire and Debris analysis, Injuries, Firearm wounds, Asphyxia and stress analysis (only analytical identifications).

## Unit III

Forensic Toxicology: Analysis of various types of poisons (corrosive, irritant, analgesic, hypnotic, tranquillizer, narcotic, stimulants, paralytic, anti-histamine, domestic and industrial (gaseous and volatile) poisoning and food poisonings), Explosive and explosion residue analysis, Lethal drug analysis (sampling, sealing, packing, laboratory methods of testing, reporting the analysis results, court evidence and medico-legal aspects for the consideration of chemical data as a proof for crime), Importance of physiological tests in forensic toxicology

## Unit IV & V

### Instrumentation for Forensic Analysis

(a) Physical, Biological and Chemical Methods: Non-destructive testing probes including radiography, Xera-radiography, Surface penetrations method (SEM and Laser Probes), Fluoroscopy, Clinical methods: ELISA, RIA and immunodiffusion , analysis of glucose, bilirubins, total cholesterol, creatinine, blood urea nitrogen and barbiturates in biological fluids, DNA-finger printing, Examination and grouping of blood strains and seminal strains, Data retrieval and automation techniques for forensic examination with reference to presence of drugs, glasses, paints, oils and adhesives at crime spot.

(b) Instrumental Methods: Sample preparation, calibration of instruments for accuracy and reproducibility of results in forensic analysis, method validation technique and requirements, procurement of standard samples, Forensic applications of TLC, HPTLC, HPLC, GC, FT-IR, AAS, GC-MS, UV-visible spectrophotometer with emphasis over standard operational procedures (SOPs) for test samples.

### **Books Suggested** (Names of Publishers may vary as per copyright status):

1. W.J. Welcher (Ed.), Scott's Standard Methods of Chemical Analysis, Vol. III A, 6<sup>th</sup> Edition (1966), and vol. III B, 5<sup>th</sup> Edition (1975), Van Nostrand Reinhold Co. London.
2. Peter Fordham, Non-destructive Testing Techniques, 1<sup>st</sup> edition (1968), London Business Publications Ltd., London
3. W. Horwitz, Official Methods of Analysis, 11<sup>th</sup> Edition (1970), Association of Official Analytical Chemists, Washington DC.
4. K. Simpson and B. Knight, Forensic Medicine, 9<sup>th</sup> Edition (1985), Edward Arnold Publishers Ltd., London.

## Concepts in Organic Synthesis (CHE-306)

### Unit I

Disconnection Approach: General introduction to synthons and Synthetic equivalents, Disconnections, (C-C, C-S, C-O, bonds), Functional group interconversion, chemoselectivity, cyclisation reaction, choosing synthetic route for small and large scale synthesis.

### Unit II

Synthetic Strategies: (a) For formation of carbon-carbon bond (b) For formation of carbon-nitrogen bond (c) Formation of carbon-halogen bond (d) Ring Synthesis and (e) Multistep Synthesis.

### Unit III

(i) Protecting Groups: Principle of protection of alcoholic, amino, carbonyl and carboxylic groups.

(ii) Stereochemistry in organic synthesis: Stereoselectivity and stereospecificity. Regioselectivity and regioselectivity: Asymmetric synthesis-Sharpless asymmetric epoxidation. An introduction to computer aided designing of organic synthesis.

### Unit IV

Reagents in Organic Synthesis:

(i) Complex metal hydrides. (ii) Gilman's reagent. (iii) Lithium diisopropyl amide (LDA). (iv) Dicyclohexylcarbodiimide (DCC). (v) 1,3-Dithiane (Reactivity Umpolung). (vi) Trimethylsilyl iodide. (vii) Tri n-butyltin hydride. (viii) Crown ethers. (ix) Merrifield resin. (x) Wilkinson's Reagent. (xi) Peterson's Synthesis (xii) Organic per acids. (xiii) Baker's yeast.

### Unit V

Selective organic name reaction and their synthetic application: (i) Stork Enamine reaction. (ii) Favorskii reaction. (iii) Ene Reaction. (iv) Barton Reaction. (v) Hofmann-Löffler-Freytag Reaction. (vi) Shapiro Reaction. (vii) Chichibabin Reaction. (viii) Robinson annulation.

Nitrogen, Sulphur and Phosphorus Ylides: Preparation and their synthetic applications.

**Books Suggested**(Names of Publishers may vary as per copyright status):

1. Organic Synthesis, Jagdamba Singh, L.D.S. Yadav, PragatiPrakashan
2. Advanced Organic Chemistry, Jagdamba Singh, PragatiPrakashan.
3. Organic Chemistry: Concepts and Applications, Jagdamba Singh, PragatiPrakashan.

4. Advanced Organic Chemistry Part B: Reaction and Synthesis, Francis A. Carey, Richard J. Sundberg, Springer.
5. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.
6. Advanced Organic Chemistry, Arun Bahl, B S Bahl, S Chand.

## Skill Development Paper

### Industry Visit (CHE-307)

Study tour/ Industrial visits of 7-15 days are proposed in and around Prayagraj/Uttar Pradesh for the students of 3<sup>rd</sup> semester. The students will make a report and give a ppt presentation in the department. The marks will be given on the basis of presentation and report.

## University Elective Paper

### Environmental Chemistry (CHE-308)

1. **Introduction to Environmental Chemistry:** Concept and scope of environmental chemistry, Environmental terminology and nomenclatures, Environmental segments, The natural cycles of environment (Hydrological, Oxygen, Nitrogen)
2. **Atmosphere:** Regions of the atmosphere, Reactions in atmospheric chemistry, Earth's radiation balance, Particles, ion and radicals in atmosphere; Chemistry of ozone layer.
3. **Hydrosphere:** Complexation in natural water and waste-water, Micro-organisms in aquatic chemical reactions, Eutrophication, Microbiology mediated redox reactions.
4. **Lithosphere:** Inorganic and organic components in soil, acid-base and ion-exchange reactions in soil, micro and macro nutrients, nitrogen pathways and NPK in soil.
5. **Chemical Toxicology:** Toxic chemicals in the environments, Impact of toxic chemicals on enzymes, Biochemical effects of arsenic, cadmium, lead, mercury, carbon monoxide, nitrogen oxides, sulphur oxides.
6. **Air Pollution:** Particulates, Aerosols, SO<sub>x</sub>, NO<sub>x</sub>, CO<sub>x</sub> and hydrocarbon, Photochemical smog, Air-quality standards
7. **Water Pollution:** Water-quality parameters and standards: physical and chemical parameters, Dissolved oxygen, BOD, COD, Total organic carbon, Total nitrogen, Total sulfur, Total phosphorus and Chlorine, Chemical speciation (Pb, As, Hg)

### Books Recommended

1. G.W. Vanloon, S.J. Duffer, *Environmental Chemistry - A Global Perspective*, Oxford University Press (2000).
2. F.W. Fifield and W.P.J. Hairens, *Environmental Analytical Chemistry*, 2nd Edition (2000), Black Well Science Ltd.
3. Colin Baird, *Environmental Chemistry*, W.H. Freeman and Company, New York (1995).
4. A.K. De, *Environmental Chemistry*, 4th Edition (2000), New Age International Private Ltd., New Delhi.
5. Peter O. Warner, *Analysis of Air Pollutants*, 1st Edition (1996), John Wiley, New York.
6. S.M. Khopkar, *Environmental Pollution Analysis*, 1st Edition (1993), Wiley Eastern Ltd., New Delhi.
7. S.K. Banerji, *Environmental Chemistry*, 1st Edition (1993), Prentice-Hall of India, New Delhi.

## *Semester III*

\*For core papers of Specializations please see at the end of the syllabus

### **Elective Papers**

#### **Physical Methods in Chemistry (CHE-404)**

##### Unit I

Photoelectron Spectroscopy and Related Techniques: Principle and applications to studies of molecules and surface. UPES and XPS. Auger electron and X-ray fluorescence spectroscopy (AES and XRF).

##### Unit II

Techniques for Studying Surface Structure: Low energy electron diffraction (LEED). Scanning tunneling and atomic force microscopy (STM and AFM).

##### Unit III

Neutron Diffraction: Principle and applications.

##### Unit IV

Fluorescence techniques: Steady-state fluorescence spectroscopy. Time-resolved (Time correlated single photon counting-TCSPC) fluorescence spectroscopy. Introduction to Single molecule fluorescence and fluorescence imaging.

**Books Suggested**(Names of Publishers may vary as per copyright status):

1. J.M. Hollas, Modern Spectroscopy, 4th edition (2004), John Wiley and Sons, Chichester.
2. C.N. Banwell and E.M. Mc Cash, Fundamentals of Molecular Spectroscopy, 4th edition (1994), Tata McGraw Hill, New Delhi.
3. E.M. Mc Cash, Surface Chemistry, Oxford University Press, Oxford (2001).
4. A.K. Cheetham and P Day, Solid State Chemistry Techniques, Oxford Univ. Press, Oxford (1988).
5. Joseph R. Lakowicz, Fluorescence Spectroscopy, 2nd edition, Plenum Press, New York. (1999).

#### **Principle and Applications of Luminescence Spectroscopy (CHE-405)**

##### Unit I

Luminescence, a brief history, different kinds of luminescence, electronic transition, transition probability, fluorescence and other de-excitation process, phosphorescence versus non-radiative de-excitation, delayed fluorescence,

##### Unit II



Basic instrumentation of steady-state and time-resolved fluorometer, characteristics of fluorescence emission, solvent and environmental effects, red-edge effects, effects of intermolecular photophysical processes on emission, static and dynamic quenching,

### Unit III

Stern-Volmer kinetics, emission anisotropy, intrinsic and extrinsic probes, chemical sensing probes, probes of analyte recognition, electron transfer probes,

### Unit IV

Energy transfer, energy transfer to multiple acceptor, biochemical applications, pH and CO<sub>2</sub> sensors, protein fluorescence and protein sensors, glucose sensors, novel fluorophores: semiconductor nano particles, lanthanides, metal-ligand complexes,

### Unit V

Long-wavelength and long-lifetime fluorophores, advanced techniques in fluorescence spectroscopy.

**Books Suggested**(Names of Publishers may vary as per copyright status):

1. J. R. Lakowicz, Principles of Fluorescence Spectroscopy, Springer, 3rd Ed. 2006.
2. B. Valuer, Molecular Fluorescence, Wiley-VCH, 2002.
3. N. J. Turro, Modern Molecular Photochemistry, University Science Books, 1991.
4. J. R. Lakowicz, Topics in Fluorescence Spectroscopy, Vol. 1: Techniques, Plenum Press, 1991.
5. J. R. Lakowicz, Topics in Fluorescence Spectroscopy, Vol. 4: Probe Design and Chemical Sensing, Kluwer Academic Press, 1994.
6. B. Valuer and J. C. Brochon, New Trends in Fluorescence Spectroscopy: Applications to Chemical and Life Sciences, Springer, 2001.

## **Advances in Nucleic Acid and Lipid Chemistry (CHE-406)**

### Unit I

Nucleic acids: Definition, structure and properties, base pairing, double helices, DNA replication, genetic information storage, transmission and gene expression,

### Unit II

Chemical synthesis of oligonucleotides, hybridization with synthetic oligonucleotides, characterization and purification techniques, nucleic acids as molecular probes.

### Unit III

DNA damages, mutations and repair. Modified nucleic acids: Peptide nucleic acids (PNAs), LNAs, synthesis of PNAs, doubly labeled PNAs as probes for the detection of point mutations.

## Unit IV

Lipids, fatty acids, bilayer, liposome, lipidation of proteins and peptides, farnesylation of the Ras protein. Synthesis of lipids. Role of lipids in drug delivery and gene delivery. Lipid probes. Biophysical properties of lipid-protein, lipid-peptide interactions.

## Unit V

Transport across membranes. Lipidated proteins and peptides in model membranes. Basic concepts of fluorescence and lipid markers. synthesis of fluorescence quencher and lipidated peptides.

**Books Suggested**(Names of Publishers may vary as per copyright status):

1. C.M. Dobson, J.A. Gerrard and A.J. Pratt., *Foundations of Chemical biology*, Oxford University Press. 2002.
2. A. Miller and J. Tanner, *Essentials of Chemical Biology*, Willey & Sons Ltd. 2008.
3. S. L. Schreiber, T. Kapoor and G. Wess, *Chemical Biology: from small molecules to systems biology and drug design*, Wiley – VCH Verlag GmbH & Co. 2007.

## Skill Development Paper

### Computer Application in Chemistry (CHE-407)

1 **FORTRAN Programming:** Types of Constants and Variables in Fortran, Dimension, Data, Type, COMMON and EQUIVALENCE statements, Arithmetic and Logical IF, IF-THENELSE constructs, 'DO' statement, Various types of 'I/O' statements, Library functions, Statement functions, Function subprograms and subroutine subprograms.

2 **Numerical Methods:** Roots of Polynomials, Solution of Linear simultaneous equations, matrix multiplication and inversion. Numerical integration. Statistical treatment of data, variance and correlations.

3. Computer programming based on FORTRAN and Numerical methods

4. Exposure to available standard application packages like: Chemdraw, generation of graphs, data sheets creation, and tables using Excel Programme.

### Books Recommended

1. V. Rajaraman, *Fortran 77*, Prentice Hall (India), New Delhi (1997)
2. C. Xavier, *Fortran 77 and Numerical Methods*, New Age International Pvt. Ltd. Publishers, New Delhi (1994)
3. S. Lipschutz and A. Poe, *Schaum's Outline Series – Theory and Problems of Programming with Fortran including structured Fortran*, Mc Graw Hill Book Company, Singapore (1982)
4. K. V. Raman, *Computers in Chemistry*, Tata McGraw Hill (1993). [Reference book]

## **University Elective Paper** **Nanochemistry (CHE-408)**

### **Unit I**

Introduction: History scope and perspectives of nanochemistry. Synthesis and Stabilization of Nanoparticles, Chemical Reduction; Reactions in Micelles, Emulsions, and Dendrimers; Photochemical and Radiation Chemical Reduction.

### **Unit II**

Experimental Techniques: Transmission and scanning electron microscopy, Probe Microscopy, X-ray diffraction, Neutron diffraction, Miscellaneous Techniques, Comparison of Spectral Techniques used for Elemental Analysis.

### **Unit III**

Size Effects in Nanochemistry: Models of Reactions of Metal Atoms in Matrices; Properties; Kinetic Peculiarities of Chemical Processes on the surface of Nanoparticles; Thermodynamic Features of Nanoparticles.

### **Unit IV**

Applications of Nanoparticle in various fundamental research, industries, medical field.

### **Unit V**

Environmental issue; toxicity, biosafety and ethical issue in applications of Nanoparticle.

**Books Suggested** (Names of Publishers may vary as per copyright status):

1. Nanomaterials and Nanochemistry, edited by C. Brechignac, P. Houdy, M. Lahmani, Springer-Verlag, Berlin.
2. Nanoparticle Technology Handbook. M. Hosokawa, K. Nogi, M. Naito, T. Yokoyama (Eds.), Elsevier.
3. Nanotechnology Basic Calculations for Engineers and Scientists, Louis Theodore, John Wiley and Sons.
4. Nanochemistry: A Chemical Approach to Nanomaterials, Geoffrey A Ozin, André Arsenault, Ludovico Cademartiri, RSC Publishing.

## **Specialization Papers**

### **Analytical Chemistry** **III SEM**

#### **PAPER – I**

#### **Analytical Chemistry-S-I (CHE-301A)**

##### **UNIT-I**

Statistical Methods in Analytical Chemistry

(a) Descriptive Statistics: Distribution of random numbers, Gaussian distribution, other distributions, Central limiting theorem; Location parameters – Arithmetic, Geometric and Harmonic means, Median, Quartile; Confidence level and Confidence interval

(b) Statistical Test: Testing hypothesis-comparison of a mean with a true value: one – variable test, comparison of two means: two variable t – test; comparison of variables F-test, Testing for distribution  $\chi^2$ - test Test for outliers – Dixons -test

(c) Statistics of Sampling

#### UNIT-II

Linear least Squares : Least Squares plot; standard deviations of the slope and intercept; Correlation coefficient and coefficient of determination

#### UNIT-III

Graphic presentation of equilibrium data: acid base, solubility and complex formation

#### UNIT-IV

Kinetic Methods of Analysis: Enzyme catalysis – Enzyme kinetics, properties of enzymes, Enzyme Inhibitors and Activators; The Michaelis constant Determination of enzymes and Example of Enzymatic Analysis.

#### UNIT-V

Concept of Speciation – Iodine Species ( $I^-$ ,  $IO_3^-$ ,  $I_3^-$  and  $I_2$ ); Actinide Speciation in Aquatic Environment, Lead, Chromium

#### Books Recommended

1. D.A. Skoog and D.M. West, Fundamental of Analytical Chemistry, International Edition, 7th Edition (1996), Saunders College Publishing, Philadelphia, Holt, London.
2. R.L. Pecsok, L.D. Shields, T. Cairns and L.C. McWilliam, Modern Methods of Chemical Analysis, 2nd (1976), John Wiley & Sons, New York.
3. D.A. Skoog, Principles of Instrumental Analysis, 5th Edition (1998), Saunders College of Publishing, Philadelphia, London.
4. H.A. Strobel, Chemical Instrumentation: A Schematic Approach, 2nd Edition (1973), Addison Wesley, Reading, Mass.

### **PAPER – II**

#### **Analytical Chemistry-S-II (CHE-302A)**

#### UNIT-I

Principles and applications of solvent extraction: quantitative treatments of extraction equilibria, solvent extraction of metals, analytical separation, multiple batch extraction, counter current distribution, synergistic extraction. Solid –phase extraction, Supramolecules in solvent extraction

#### UNIT-II

Ion exchange Resins – Mechanism of ion exchange, synthesis and characteristics of ion-exchange resins, Factors affecting the selectivity of ion exchange resin, Ion exchange capacity, Techniques in ion exchange methods and analytical applications.

#### UNIT-III

Ion Chromatography – Ion chromatography as a separation tool, Instrumentation in Ion chromatography; Analytical Applications of Ion chromatography Adsorption chromatography:– Principle, Experimental Set up and use of Adsorption chromatography

#### UNIT-IV

Partition Chromatography- Principle of Liquid – Liquid partition chromatography Reversed Phase Partition chromatography, Application of Extraction Chromatography, Paper, Thin Layer and Ion-pair chromatography

#### UNIT-V

Electrophoresis – Principles of Electrophoresis – Classification of Electrophoresis Methods, Techniques of Electrophoresis and Instrumentation, Applications in Inorganic Chemistry, Separation of Biological Products.

#### Books Recommended

1. G.H. and H. Freiser, Solvent Extraction in Analytical Chemistry, 1st Edition (1958), John Wiley, New York.
2. B.L. Karger, L.R. Snyder and C. Howarth, An Introduction to Separation Science, 2<sup>nd</sup> Edition (1973), John Wiley, New York.
3. E.W. Berg, Chemical Methods of Separation, 1st Edition (1963), McGraw Hill, New York.
4. D.G. Peters, J.M. Hayes and C.M. Hieftj, Chemical Separation and Measurements, 2<sup>nd</sup> Edition (1974), Saunders Holt, London.
5. J.D. Seader and E.J. Henley, Separation Process Principles, 1st Edition (1998), John Wiley & Sons. Inc., New York.

## **PAPER – III**

### **Analytical Chemistry-S-III (CHE-303A)**

#### UNIT-I

Turbidimetry and Nephelometry and their applications Fluorometry – Principle of Fluorescence, Chemical Structures and Fluorescence, Relationship between concentration and Fluorescence Intensity, Fluorescence Instrumentation

#### UNIT-II

Flame Emission Spectroscopy : Principles of Flame Photometry, Instrumentation Evaluation Methods in Flame Photometry

#### UNIT-III

Atomic Absorption Spectrophotometry (AAS) : Principles, Instrumentation, Interferences, Sample preparation, Applications of AAS, Sensitivity and Detection Limits in Analysis, Graphite Furnace in AAS

#### UNIT-IV

Inductively Coupled plasma Atomic Emission Spectroscopy : Limitation of Flame Emission spectroscopy, Principles of plasma spectroscopy, Inductively coupled Plasma Source, ICP-AES Instrumentation, Applications of Plasma Spectroscopy

#### UNIT-V

Principles of Infrared Spectrophotometry and Raman Spectroscopy, FT-IR and FT Raman Spectrometers, Applications of these techniques in Quantitative analysis.

#### Books Recommended

1. P.L. Kirk, Quantitative Ultramicroanalysis, John Wiley.
2. C.L. Wilson and D.L. Wilson, Comprehensive Analytical Chemistry”, Vol. I (A) and I(B), Elsevier.
3. G.D. Christian, Analytical Chemistry, John Wiley & Sons, New York (2001).
4. S.M. Khopkar, Analytical Chemistry of Macrocyclic and Supramolecular Compounds, Narosa Publishing House, New Delhi (2002).
5. Jag Mohan, Organic Analytical Chemistry - Theory and Practice, Narosa Publishing House, New Delhi (2003).

## **Analytical Chemistry Laboratory**

1. Separation of  $Zn^{2+} + Mg^{2+}$  present in a sample using anion exchange resin and estimation of each metal ion thus separated by E.D.T.A. titration.
2. Separation of  $Co^{2+} + Ni^{2+}$  present in a sample using anion exchange resin and estimation of each metal ion thus separated by E.D.T.A. titration.
3. Determination of the pH of Hair shampoos.
4. Determination of the  $pK$  value of weak organic acid by pH titration.
5. U.V. Spectrophotometric determination of Aspirin, Phenacetin and Caffeine in APC tablets using solvent extraction Determination of Fe(III) by chloride extraction in ether
6. Separation of amino acids using paper chromatography
7. Electrophoresis
8. Flame emission photometric determination of sodium
9. Infrared determination of a mixture of Xylene isomers / APC tablet
10. Thin – Layer chromatography, Separation of Amino acids.
11. Water analysis

## **IV SEM**

### **Paper IV**

#### **Analytical Chemistry-S-IV (CHE-401A)**

##### **UNIT- I**

Voltametry : The voltametric cell, the current voltage curve, the step wise reduction or oxidation supporting electrolyte chemicals modified electrodes.

##### **UNIT- II**

Polarography: The dropping mercury electrode, concepts of half wave potential, residual current, maxima, the Ilkovic equation, Ac polarography, Rapid scan Polarography, Square wave polarography, Inorganic and organic Polarography.

### UNIT- III

Anodic stripping voltametry, cyclic voltametry squarewave polarography, chronopotentiometry.

### UNIT- IV

Chemical Sensors classification, sensitivity and limit of detection, potentiometric sensors Ion selective Electrodes (ISEs), types of electrodes, selectivity and applications of ISEs., Gas sensors, voltametric sensors

### UNIT- V

Biosensors – Definition, The enzyme electrode, biosensors based on Ion-Selective electrodes, amperometric enzyme electrodes, applications of enzyme electrodes; Biosensors based on plant and animal tissue.

#### Books Recommended

1. L. Meites, Polarographic Techniques, 2nd Edition (1965), John Wiley, New York.
2. J. Heyrovsky and K. Kuta, Principles of Polarography, 1st Edition (1966), Academic Press, New York.
3. D.A. Skoog, F.J. Holler and T.A. Nieman, Principles of Instrumental Analysis, 5th Edition (1998), Saunders College Publishing, Harcourt Brace & Company, U.S.A.
4. A.J. Bard and L.R. Faulkner, Electrochemical Methods: Fundamentals and Applications, 2nd Edition (2000), Wiley, New York.

#### Additional References

1. I.M. Kolthoff and J.J. Lingane, Polarography, 2nd Edition (1952), Wiley Intersciences, New York.
2. C.W.C. Milner and G. Phillips, Coulometry in Analytical Chemistry, Pregamon Press, New York (1967).

## **Paper V**

### **Analytical Chemistry-S-V (CHE-402A)**

### UNIT- I



Thermal and calorimetric methods of Analysis : Thermogravimetric Analysis (TGA) – Principle, apparatus and applications; Differential Thermal analysis (DTA) – Principle and apparatus; Derivative thermogravimetry – principle and apparatus, Interpretation of TGA and DTA curves. Thermometric titrations; Differential scanning calorimetry (DSC) - Instrumentation and Applications

#### UNIT- II

X-ray Emission Spectrometry : X-ray processes, X-ray Fluorescence, X-ray fluorescence Spectrometer, Applications of X-ray emission spectrometry.

#### UNIT- III

Mass spectrometry : Principles, Basic idea of techniques and applications Gas chromatography and High Performance Liquid Chromatography : Principle, Instrumentation and Applications.

#### UNIT- IV

Polarimetry and Related methods: Polarised Light, Applications of Polarimetry, Optical Rotatory Dispersion (ORD) and Circular Dichromism (CD), Instrumentation for ORD and CD.

#### UNIT- V

The role of computers and microprocessors in Analytical Chemistry- Instrument optimizations, Data recording and storage, Data processing and data analysis (Chemometry), The scope of microprocessor Control and computers in analytical laboratories.

#### Books Recommended

1. D.A. Skoog, F.J. Holler and T.A. Nieman, Principles of Instrumental Analysis, 5th Edition (1998), Harcourt Brace & Company, Florida.
2. R.L. Pecsok, L. D. Shields, T. Cairns and L.C. Mc William, Modern Methods of Chemical Analysis, 2nd Edition (1976), John Wiley, New York.
3. J.M. Hollas, Modern Spectroscopy, 3rd Edition (1996), John Wiley, New York.
4. H.A. Strobel, Chemical Instrumentation – A Systematic Approach, 2nd Edition (1973), Addison Wesley, Mass.

5. D.C. Garratt, the Quantitative Analysis of Drugs, 2nd Edition (1992), Chapman and Hall Ltd., London.

6. W. Horwitz (Editor), Official Methods of Analysis, 11th Edition (1970), Association of Official Analytical Chemists, Washington DC.

## **Paper VI**

### **Analytical Chemistry-S-VI (CHE-403A)**

#### UNIT- I

Miscellaneous Analysis Determination of moisture by Karl Fischer's method and active hydrogen by Zerwintinoff's method

#### UNIT- II

Gas Analysis – Volumetric methods of analysis of gases, determination to H<sub>2</sub>O<sub>2</sub> (?), determination of available chlorine in bleaching powder.

#### UNIT- III

Analysis of oils and fats. Acquaintance with commercial analysis of food materials like milk, butter, tea, sugar and vitamins.

#### UNIT- IV

Micro and Semi-micro determinations of functional groups like amino, nitro, azo, carbonyl, unsaturation, acetylenic hydrogen, sulphonic acid, sulphide, sulphamide and peroxides

#### UNIT- V

Micro and semi-micro determination of oxygen, phosphorus, arsenic and halogens (including fluorine in organic compounds).

#### Books Recommended

1. Fundamentals of Analytical Chemistry, D.A. Skoog, D.M. West and F.J. Holler, W.B. Saunders.
2. Analytical Chemistry-Principles, J. H. Kennedy, W.B. Saunders.
3. Analytical Chemistry-Principles and Techniques, .G. Hargis, Prentice Hall.
4. Principles of Instrumental Analysis, D.A. Skoog, W. B. Saunders.
5. Instrumental methods of chemical analysis by B K Sharma Goel publishing House Ltd

6. Essentials of Nuclear chemistry HJ Arnikaar, Wiley eastern.
7. D. A. McQuarrie, Quantum Chemistry (University Science Books, Mill Valley, CA,).
8. P. W. Atkins. Molecular Quantum Mechanics, Oxford Univ. Press

## **Inorganic Chemistry**

### **III SEM**

#### **Paper I**

#### **Inorganic Chemistry-S-I (CHE-301I)**

##### UNIT-I

Role of Metal Ions in Biological Systems: Photosystems; nitrogen fixation, Na<sup>+</sup> / K<sup>+</sup> pump.

##### UNIT-II

Complexes of Biological Significance: Metal complexes of porphyrins and phthalocyanin, Vitamin B<sub>12</sub> and B<sub>6</sub>; chlorophylls.

##### UNIT-III

Metallo Proteins: Function, Electronic structure, bonding and stereochemistry of the active site –

(1) Natural oxygen carrying proteins – Haemoglobin, Myoglobin, Hemerythrins and Hemocyanin

(2) Electron Transport Protein – (a) Iron – sulfur Proteins – Rubredoxin and Ferredoxins (b) Cytochromes (types a, b and c)

##### UNIT-IV

Metallo enzymes –

Mo-containing Enzymes – Nitrogenase; Xanthine Oxidase, sulphite, Oxidase and Nitrate reductase (b) Iron-containing Enzymes – cytochrome – c- oxidase, catalases, Peroxidases, cytochrome-p-450

##### UNIT-V

Copper – containing Enzymes – Superoxide dismutase (SOD), Bovine Superoxide dismutase (BOD), ascorbic acid oxidase and (b) Zinc – containing Enzymes carboxy – peptidase A and B; carbonic anhydrase and Urease.

#### Books Recommended

1. M. N. Hughes, Inorganic Chemistry of Biological Processes, 2nd Ed.(1981), John-Wiley & Sons, New York.
2. W. Kaim and B. Schwederski, Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, An Introduction and Guide, Wiley, New York (1995).
3. S. J. Lippard and J. M. Berg, Principles of Bioinorganic Chemistry, University Science Books, (1994).
4. I. Bertini, H. B. Grey, S. J. Lippard and J. S. Valentine, Bioinorganic Chemistry, Viva Books Pvt. Ltd., New Delhi (1998)

## **Paper II**

### **Inorganic Chemistry-S-II (CHE-302I)**

#### UNIT-I

Classification of organometallic compounds based on hapticity and polarity of M-C bond; Nomenclature and general characteristics.

#### UNIT-II

Complexes of  $\sigma$ -Donor  $\pi$  -donor Organic Ligands Transition metal alkenyls, alkynyls, carbenes and carbenes. Preparation, bonding and structure of alkene, alkyne, allyl, dienyl and arene complexes, important reactions with special reference to nucleophilic and electrophilic attack on ligands and to organic synthesis.

#### UNIT-III

Transition Metal Compounds in Homogeneous Catalysis and compounds with M-H bond Hydrogenation, hydroformylation and Zeigler-Natta polymerization of olefins.

#### UNIT-IV

Wacker Process, hydrocarbonylation of olefins, oxopalladation reactions, activation of C-H bond. Metal hydrides (classical and non-classical).

#### UNIT-V

Fluxional Organometallic Compounds Fluxional alloy and dynamic equilibria in compounds such as  $n^2$  – olefins and  $n^3$  – allyl and diene complexes.

#### Books Recommended

1. F.A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, 6th Ed. (1999) John Wiley & Sons, NY.
2. J.E. Huheey, Keiter and Keiter, Inorganic Chemistry, YEAR?
3. R. H. Crabtree, The Organometallic Chemistry of Transition Metals, John Wiley. YEAR?
4. Ch. Elschenbroich and A. Salzer, Organometallics, VCH. YEAR?
5. J.P. Collman, L.S. Hegedus, J.R. Norton and R.G. Finke, Principles and Applications of Organotransition metal Chemistry, Univ. Sci. Books, Mill Valley. California. YEAR

### **Paper III**

#### **Inorganic Chemistry-S-III (CHE-303I)**

##### UNIT-I

Coordination Polymers: Classification, types of metal-organic frameworks (MOFs), Synthetic strategies, characterization, properties and applications.

##### UNIT-II

Metal Carbonyls and related Compounds: Preparation structure and properties; bonding in metal carbonyls, variants of CO bridging vibrational spectra of metal carbonyls, principle reaction types of metal carbonyls, metal nitrosyl.

##### UNIT-III

Polyhedral Boranes: Higher boranes, carboranes, metallo-boranes and metallo-carboranes – Structure and bonding in the light of Wade's and Jemmis' Rules.

##### UNIT-IV

Synthesis and applications of nanoparticles: Introduction of Nano Particles; its different methods for preparation; its applications to chemistry.

##### UNIT-V

Alkoxides Properties; structural aspects of various types of alkoxides – Industrial applications and catalytic aspects of metal alkoxides.

## Books Recommended

1. F. A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, 6th Edn. (1999), John-Wiley & Sons, New York.
2. James E. Huheey, Inorganic Chemistry, 4th Edn. (1993), Addison Wesley Pub. Co., New York
3. N. N. Greenwood and A. Earnshaw, Chemistry of the Elements, 2nd Edn. (1997), Butterworth Heinemann, London.

## **Inorganic Chemistry Laboratory**

Separation of a Mixture of Cations/Anions by Paper Chromatographic

Technique Using Aqueous/Non-aqueous Media:

- a.  $\text{Pb}^{2+}$  and  $\text{Ag}^+$  (aqueous and non-aqueous media)
- b.  $\text{Co}^{2+}$  and  $\text{Cu}^{2+}$  (non aqueous media)
- c.  $\text{Cl}^-$  and  $\text{I}^-$  (aqueous – acetone media)
- d.  $\text{Br}^-$  and  $\text{I}^-$  (aqueous – acetone media)

Ion-exchange Method of Separation

- e. Separation of  $\text{Zn}^{2+}$  and  $\text{Mg}^{2+}$  on an anion exchanger
- f. Separation of  $\text{Co}^{2+}$  and  $\text{Ni}^{2+}$  on an anion exchanger

## **IV SEM**

### **Paper IV**

#### **Inorganic Chemistry-S-IV (CHE-401I)**

#### UNIT- I

NMR Spectroscopy (i) : Use of Chemical shifts and spin-spin couplings for structural determination; Double resonance, and Dynamic processes in NMR; Decoupling phenomenon, Nuclear Overhauser Effect, DEPT spectra and structural applications in

$^{13}\text{C}$ NMR; Use of Chemicals as NMR auxiliary reagents (shift reagents and relaxation reagents);  $^1\text{H}$  NMR of paramagnetic substances.

#### UNIT- II

Nuclear Spectroscopy – (ii) Multinuclear NMR of Metal nuclei.  $^{31}\text{P}$ ,  $^9\text{F}$ ,  $^{27}\text{Al}$ ,  $^{11}\text{B}$ ,  $^{119}\text{Sn}$ ,  $^{203/205}\text{Tl}$ ,  $^{51}\text{V}$  etc.

#### UNIT- III

Electron Spin Resonance Spectroscopy: Basic principle, Hyperfine Splitting (isotropic systems); the g value and the factors affecting thereof; interactions affecting electron energies in paramagnetic complexes (Zero-field splitting and Kramer's degeneracy); Electron-electron interactions, Anisotropic effects (the g value and the hyperfine couplings); Structural applications of transition metal complexes.

#### UNIT- IV

Infrared and Raman Spectroscopy: Basic Principle, Fundamental modes, Factors affecting vibrational frequency, Applications of vibrational spectroscopy in investigating (i) symmetry and shapes of simple  $\text{AB}_2$ ,  $\text{AB}_3$  and  $\text{AB}_4$  molecules on the basis of spectral data, (ii) mode of bonding of ambidentate ligands (thiocyanate, nitrate, sulphate and ureas).

#### UNIT- V

Mass Spectrometry: Basic Principle, Fragmentation pattern and Fingerprint applications in the interpretation of Mass spectra, effect of isotopes on the appearance of mass spectrum, recognition of the molecular ion peak; Ionization techniques (ESI, TOF and FAB)

#### Books Recommended

1. E. A. V. Ebsworth, D. W. H. Rankin and S. Craddock, Structural Methods in Inorganic Chemistry, 1st Edn.(1987), Blackwell Scientific Publications, Oxford, London.
2. R. S. Drago, Physical Methods in Chemistry, International Edition (1992), Affiliated East-West Press, New Delhi.
3. K. Nakamoto, Infrared and Raman Spectra of Inorganic and Coordination Compounds, 4<sup>th</sup> Edn. (1986), John Wiley & Sons, New York.
4. W. Kemp, Organic Spectroscopy, 3rd Edn. (1991), Macmillan, London.

5. G. Aruldas, Molecular Structure and spectroscopy, Prentice Hall of India Pvt. Ltd., New Delhi (2001).

## **Paper V**

### **Inorganic Chemistry-S-V (CHE-402I)**

#### UNIT- I

Magnetic Properties: Magnetic behaviours, recent methods of magnetic susceptibility measurements, anomalous magnetic properties of transition metal complexes, spin crossover phenomena, magnetic properties of binuclear metal complexes involving metal-metal exchange interaction (Bleaney- Bower equation).

#### UNIT- II

X-ray Photo electron Spectroscopy and Related Techniques: Basic principles, spectral features and their applications to structural determination of inorganic molecules and metal complexes: X-ray Photoelectron Spectroscopy (XPS), Auger Electron Spectroscopy (AES).

#### UNIT- III

X-Ray Spectroscopy : X-ray Absorption Fine Structure Spectroscopy (EXAFS and XANES) with synchrotron radiations techniques and X-ray fluorescence (XRF).

#### UNIT- IV

UV Visible Spectroscopy: Theory and its applications to metal complexes

#### UNIT- V

Mossbauer Spectroscopy: Basic principle, conditions for Mossbauer spectroscopy, spectral parameters (Isomer shift, electric quadrupole interactions, magnetic interactions), temperature dependent effects, structural deductions for iron and tin – complexes, miscellaneous applications. Nuclear Quadrupole Resonance (NQR) – Theory and its applications.

## **Paper VI**

### **Inorganic Chemistry-S-VI (CHE-403I)**

#### UNIT- I



(i) Electron Microscopy: SEM (Scanning electron microscopy), and TEM (Transmission electron microscopy).

#### UNIT- II

(ii) Electron Microscope AFM (Atomic force microscopy) STM (Surface tunneling microscopy).

#### UNIT- III

Photochemistry of Transition Metal complexes: Photoreactions of inorganic complexes.

#### UNIT- IV

Electrochemical Methods: Cyclic voltammetry.

#### UNIT- V

Differential pulse voltammetry, anodic stripping voltammetry, chronoamperometry, coulometry.

## **Organic Chemistry III SEM**

### **PAPER-I**

#### **Organic Chemistry-S-I (CHE-3010)**

#### UNIT-I

**Molecular Rearrangements:-** Migration to electron deficient carbon atom: Pinacole-Pinacolone rearrangement, Wagner-Meerwein rearrangement, Tiffeneau-Demjanov ring expansion, Dienone-Phenol rearrangement, Benzil Benzilic acid rearrangement, Favorski rearrangement.

#### UNIT-II

Migration to electron deficient nitrogen atom: Wolf, Hofmann, Curtius, Losen, Schmidt, Beckmann rearrangement.

Migration to electron deficient oxygen atom: Baeyer-Villiger rearrangement.

#### UNIT-III

Photochemistry of Carbonyl Compounds: Photochemistry of enones, hydrogen abstraction.

#### UNIT-IV

Rearrangements of  $\alpha$ ,  $\beta$  - unsaturated ketones and cyclohexadienones, photochemistry of p-benzoquinones.

#### UNIT-V

Photochemistry of unsaturated system: Olefins, cis-trans isomerisation, dimerisation, hydrogen abstraction and additions. Acetylenes-dimerisation, Dienes-photochemistry of 1, 3-butadiene (2+2) additions leading to cage structures, photochemistry of cyclohexadienes, Photochemistry of aromatic compounds-excited state of benzene and its 1,2 and 1, 3-shifts, Photo-Fries rearrangement, Photo-Fries reaction of anilides, photosubstitution reaction of benzene derivatives, Photolysis of nitride esters and Barton reaction.

## **PAPER – II**

### **Organic Chemistry-S-II (CHE-302O)**

#### UNIT-I

Oxidation: Hydrocarbons-alkenes, aromatic, rings, saturated, C-H groups (activated and unactivated), alcohols, diols.

#### UNIT- II

Aldehydes, ketones and carboxylic acids, amines, hydrazines and sulphides. Oxidations with ruthenium tetroxide, iodobenzene diacetate and thallium (III) nitrate.

#### UNIT-III

Reduction: Hydrocarbons –alkenes, alkynes and aromatic rings. Carbonyl Compounds: aldehydes, ketones, acids and their derivatives. Epoxides; Hydrogenolysis

#### UNIT-IV

Organometallic Reagents: Synthetic applications of organometallic compounds with mechanistic details of following metals.

Hg, Cd, Ce, Cu, Ni, Fe, Co, Rh, Cr and Ti

#### UNIT- V

Application of Pd(0) and Pd(II) complexes in organic synthesis – Stille, Suzuki and Sonogashira coupling, Heck reaction and Negishi coupling.

## PAPER III

### Organic Chemistry-S-III (CHE-3030)

#### UNIT-I

**Disconnection Approach:** General introduction to synthons and Synthetic equivalents, Disconnections, (C-C, C-S, C-O, bonds).

#### UNIT-II

Functional group interconversion, chemoselectivity, cyclisation reaction choosing synthetic route for small and large scale synthesis.

#### UNIT-III

**Protecting Groups:** Principle of protection of alcoholic, amino, carbonyl and carboxylic groups.

#### UNIT-IV

Stereochemistry in Organic Synthesis: Stereoselectivity and stereospecificity. Regioselectivity and regiospecificity: Asymmetric synthesis- Sharpless asymmetric epoxidation.

#### UNIT-V

##### **Synthetic Strategies:**

- (i) For formation of carbon-carbon bond.
- (ii) For formation of carbon-nitrogen bond.
- (iii) For formation of carbon-halogen bond.
- (iv) For Ring Synthesis
- (v) For Multistep Synthesis

#### **Organic Chemistry Laboratory**

- (a) Separation and identification of organic compounds using chemical methods from organic mixtures containing up to three components
- (b) Preparation of organic compounds involving several stages

- (c) Verification of Lambert Beer's Law using bromocresol green reagent.
- (d) Estimation of carbohydrates, protein, amino acids, ascorbic acid, blood cholesterol and aspirin in APC tablets by UV-Visible spectrophotometric method.

## IV SEM

### Paper IV (Biosynthesis and Chemistry of Natural Products)

#### Organic Chemistry-S-IV (CHE-4010)

##### UNIT- I

##### **Bio-synthesis of Natural Products**

- (a) The acetate hypothesis, poly  $\beta$ -Ketoacids, Biosynthesis, Biogenesis Primary and Secondary reactions involved in biosynthesis. Biosynthesis of poly- $\beta$ -ketoacid
- (b) Isoprene rule, mevalonic acid from acetyl Co-enzyme A. Biosynthesis of mono, sesqui, di and triterpenes.
- (c) Shikimic acid pathway for biosynthesis of aromatic ring.
- (d) General biosynthesis of alkaloids.

##### UNIT- II

**Terpenoids and Carotenoids:** Classification, isoprene rule. Structure determination, stereochemistry, synthesis of the following representative molecules: citral,  $\alpha$  terpenol, farnesol, santonin, abietic acid and  $\beta$ -carotene, menthol. For structure elucidation emphasis is to be placed on the use of spectral data wherever possible.

##### UNIT- III

**Alkaloids:** General methods of structure elucidation, degradation, classification based on nitrogen heterocyclic ring, Structure, stereochemistry and synthesis of the following: Ephedrine, (+) nicotine, quinine and morphine. For structure elucidation emphasis is to be placed on the use of spectral data wherever possible.

##### UNIT- IV

**Steroids:** Basic skeleton Diel's hydrocarbon and stereochemistry, structure determination and synthesis of cholesterol, testosterone, estrone and progesterone. For structure elucidation emphasis is to be placed on the use of spectral data wherever possible.

UNIT- V

**Prostaglandins:** Occurrence, nomenclature, classification. Synthesis of PGE<sub>2</sub> and PGF<sub>2a</sub>

**Plant Pigments:** General methods of structure determination, synthesis of Apigenin, Quercetin Cyanidin Hirsutin. Quercetin-3 glucoside, Diazein and cyanidine-7 glucoside. For structure elucidation emphasis is to be placed on the use of spectral data wherever possible.

## PAPER V

### Organic Chemistry-S-V (CHE-4020)

UNIT- I

i. Diastereoselective,  $\pi$ - facial addition of nucleophilic to chiral carbonyl compounds: Cram's model and Felkin-Ann model

ii. Stereoselective synthesis, Asymmetric synthesis: the principle of asymmetric synthesis. Achiral substrate modified by chiral auxiliary Prelog's rule

UNIT- II

Asymmetric synthesis by the use of

i. Chiral substrate having prochiral unit

ii. Chiral auxiliary

iii. Chiral reagents

UNIT- III

Stereochemistry of some reaction

i. Mc-Murry reaction.

ii. Corey-Winter reaction.

iii. Fragmentation reaction.

iv. Wittig and related reaction.

v. Julia olefination.

#### UNIT- IV

Stereochemistry of some reaction

i. Conjugate addition with  $R_2CuLi$

ii. Mitsunobu reaction.

iii. Stereochemistry of Pd catalyzed coupling reaction

iv. Addition of Bromine and Peroxide on Cyclohexene.

#### UNIT- V

**Vitamins:** Structure determination including synthesis of

Thiamine (Vitamin B1)

Pyridoxine (Vitamin B6)

Biotin (Vitamin H)

Vitamin E

## **PAPER VI (Spectroscopy and Biomolecules)**

### **Organic Chemistry-S-VI (CHE-4030)**

#### UNIT- I

PMR Spectroscopy

Basic principles. Introduction to NMR techniques. CW and FT NMR techniques.  $^1H$  NMR Spectral parameters – intensity, chemical shift, multiplicity, coupling constant. Analysis of first order and second - order spectra. Structure determination of organic compounds by  $^1H$  NMR spectra. Problems based on PMR spectroscopy

#### UNIT- II

$^{13}C$  NMR Spectroscopy:

General considerations, chemical shift (aliphatic olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbon), coupling constants. Two dimension NMR spectroscopy-COSY, NOESY, DEPT, HMBC and HMQC techniques. Problems based on  $^{13}C$  NMR.

### UNIT- III

#### Mass Spectroscopy:

Introduction ion production. Factors affecting fragmentation, ion analysis, ion abundance  
Mass spectral fragmentation of organic compounds, common functional groups, molecular  
ion peak, metastable peak. Mc Lafferty rearrangement. Nitrogen rule. High resolution mass  
spectrometry and problems based on it.

### UNIT- IV

Antibiotics: Synthesis of penicillin G, chloramphenicol, cephalosporin, tetracycline and  
streptomycin

### UNIT- V

Pyrethroids and Rotenones, Pheromones: Synthesis and reactions of Pyrethroids and  
Rotenones. (For structure elucidation, emphasis is to be placed on the use of parameters  
wherever possible)

## **Physical Chemistry III SEM PAPER-I**

### **Physical Chemistry-S-I (CHE-301P)**

#### UNIT-I

Distribution law (Barometric formula), Sedimentation equilibrium, Maxwell's law of  
distribution of velocity and energy, Maxwell's law and Gaussian density function, R,M,S,  
Mean and Most probable velocities, Collision frequency, Collision between like and unlike  
molecules, Triple collision.

#### UNIT-II

Viscosity, thermal conductivity and diffusion coefficient of gases (quantitative treatment),  
mean free path.

#### UNIT-III

Indistinguishability of gas molecules, Maxwell-Boltzmann law for gaseous system,  
Thermodynamic functions for gaseous systems, Molar heat capacity of gases, Heat capacity

of hydrogen at low temperatures, Heat capacities of monoatomic crystals, The Einstein model, Debye's theory of solid, Heat capacities of crystals at very low temperatures.

#### UNIT-IV

Calorimetric entropy, Spectroscopic entropy, Comparison of calorimetric and Spectroscopic entropies, Third law of thermodynamics (i) Nernst Heat Theorem (ii) Entropy of chemical reactions (iii) statements of third law of thermodynamics and (iv) Conventional entropies, Expression of equilibrium constant in terms of partition functions, Equilibrium constants of simple system-(i) Ionization of metal atoms, (ii) Dissociation of diatomic molecules and (iii) Isotopic exchange equilibria.

#### UNIT-V

Calculation of thermodynamic properties from spectroscopic data, Bose-Einstein Statistic, Fermi Dirac Statistics, Comparison of M-B, B-E and F-D statistics, Fermi-Dirac gas (Electron gas in metals)- Bose—Einstein gas (liquid Helium).

## **PAPER – II**

### **Physical Chemistry-S-II (CHE-302P)**

#### UNIT-I

Magnetic susceptibility and its determination, susceptibility equivalents, Pascal's law and its applications, Diamagnetism of elements, Compounds and its ions, Langevin's theory of paramagnetism, Curie's law, Weiss molecular field theory of paramagnetism, Curie- Weiss law, Determination of Curie point.

#### UNIT-II

Orbital and spin moments, Electrons and multielectron systems, Magnetic property of complex compound in relation to their structure, Bohr magneton, L-S and J-J couplings. Electronic spectra of molecules, Born-Oppenheimer approximation, Franck-Condon principle, Rotational fine structure of Electronic-Vibration transitions, Predissociation spectra, Molecular photoelectron spectroscopy (PES).

#### UNIT-III



Quantum theory of Raman Spectra, Stokes and Antistokes lines, Rotation and vibration Raman spectra, Mutual exclusion principle, Laser Raman spectra, Theory of NMR relaxation process and chemical shift, The coupling constant, Nuclear spin interaction, Principle of ESR, Magnetic moment of electron and splitting factor, Hyper-fine splitting and double resonance in ESR.

#### UNIT- IV

Mossbauer spectroscopy and its principle, Origin of line width, Isomer shift, Quadropole effects, Application of Raman, ESR, NMR and Massbauer spectra,  $C^{13}$  NMR spectroscopy,  $P^{31}$  NMR spectroscopy STM (Scanning Tunneling Microscopy)-theory and application, AES (Auger Electron Spectroscopy), EELS (Electron Energy Loss Spectroscopy)

#### UNIT-V

Mechanism of electrode reactions, Overpotential, The current-potential relation, The Tafel equation, Hydrogen overvoltage and decomposition potential, Butler-Volmer equation,  $H_2$ -Evolution mechanism

### **PAPER III**

#### **Physical Chemistry-S-III (CHE-303P)**

##### UNIT-I

Kinetics of fast reactions: Techniques of study of fast reactions with reference to stop flow, T-Jump, Flash photolysis and relaxation phenomena. Kinetics of oscillating reactions with special reference to Belousov-Zhabotinskii mechanism (B-Z mechanism).

##### UNIT- II

Thermodynamic functions for non-equilibrium states, Postulates and methodology, Linear laws, Gibbs equation, Entropy production and entropy flow, Phenomenological equations, Microscopic reversibility and Onsager's reciprocity relations.

##### UNIT-III

Transformations of the generalized fluxes and forces, Electrokinetic phenomena, Diffusion, Electric conduction, The stationary non-equilibrium states, States of minimum entropy production.

#### UNIT-IV

Nature of intermolecular forces, Linear oscillating dipoles, Various contributions of intermolecular forces, London theory of dispersion forces, Partition function for system of independent particles, Thermodynamics of atomic crystals

#### UNIT-V

Partition function for system of dependent particles, partition functions (pressure, free energy and fugacity) of imperfect gas, Generalized model of imperfect gas and L-J potential and evaluation of second virial coefficient.

### **Physical Chemistry Laboratory**

1. Oxidation of diols by cerium(IV) sulphate in acidic medium catalyzed by rhodium(III) chloride.
2. Kinetics of oxidation of ketones by Ce(IV) sulphate in acidic medium catalysed by Ir(III) chloride .
3. Uncatalyzed and/or iridium (III) catalyzed oxidation of arsenic (III) with alkaline hexacyanoferrate (III).
4. Determination of viscosity and density of aqueous solution of glucose/sucrose/urea at different temperatures and to calculate apparent and partial molar volume.
5. Determination of molecular weight of some electrolytes and nonelectrolytes cryoscopically.

### **IV SEM**

### **Paper IV**

### **Physical Chemistry-S-IV (CHE-401P)**

#### UNIT- I

Thermodynamics:

Brief resume of concepts of laws of thermodynamics, free energy, chemical potential and entropies. Partial molar free energy, partial molar volume and partial molar heat content and their significance. Determinations of these quantities. Concept of fugacity and determination of fugacity.

#### UNIT- II

Non-ideal systems: Excess functions for non-ideal solutions. Activity, activity coefficient, Debye Huckel theory for activity coefficient of electrolytic solutions; determination of activity and activity coefficients; ionic strength. Application of phase rule to three component systems; second order phase transitions. Nernst heat theorem and its application to non-condensed systems. Statements of the third law of thermodynamics. Derivation of unattainability of absolute zero. The relationship between entropy constant and Nernst chemical constant. Applications of the third law.

#### UNIT- III

Ideal and non-ideal solutions, Inter-connection between Raoult's law and Henry's Law, Determination of Partial Molar Properties, Thermodynamic functions of mixing of nonideal solutions, Excess thermodynamic functions.

#### UNIT- IV

Gibbs-Duhem-Margules equation and its applications, Activity and activity coefficients, Activity coefficients from excess thermodynamic functions, The theory of Van Laar, Scatchard Hildebrand theory, Wilson model and Flory-Huggins theory.

#### UNIT- V

Properties of colloids, sol-Gel transformation formation, colloidal electrolytes, Micellization and surfactants.

### **PAPER V**

#### **Physical Chemistry-S-V (CHE-402P)**

#### UNIT- I

Lattice energy of crystals, Cohesive energy, Conduction in solids and superconductance, Electronic structures of solids, Free electron theory, Fermi-gas theory and band theory of solids, Metals, semi-conductors and insulators, Intrinsic extrinsic p-type and n-type semi-conductors,

## UNIT- II

Vapour pressure, compressibility viscosity and sound velocity, Internal pressure and its determination, Significance of internal pressure, solubility parameter and cohesive energy-density, Free volume of liquids and its determination, Application of free volume and its relation with energy and heat of vaporization.

## UNIT- III

Partition function of a liquid, Equation of state in terms of partition function, Outline of the theory of liquid state: Simple cell theory (Eyring equation) and cell model theory of Lennard-Jones and Devonshire, Eyring's free volume theory of liquid viscosity, Effect of pressure on viscosity, Thermodynamic functions of ideal and non-ideal liquid mixtures, Partial molar properties of liquid mixtures, Determination of partial molar volume and partial molar enthalpy,

## UNIT- IV

The triumph and limitations of Debye-Huckel theory of activity coefficients, Electrical potential and mean activity coefficient in the case of ionic clouds with finite sized ions, The ion size parameter and comparison of the finite-ion-size model with experiment, Asymmetry and electrophoretic effects, Stoke's law and Walden product, Debye-Huckel- Onsager equation, Conductance ratio and the Onsager slope, Verification of Debye- Huckel-Onsager equation, Conductivity of weak electrolytes and conductance in nonaqueous solvents, Modifications of Debye-Huckel-Onsager equation, Fuoss-Onsager and other equations, Wien and Debye-Falkenhagen effects.

## UNIT- V

Viscosity of electrolyte solutions-Jones-Dole equation and significance of A and B coefficients, Ion association in an electrolyte solution, Formation of pairs, triplets etc, The probability of finding oppositely charged ions near each other, Bjerrum theory of ion association.

## **PAPER VI**

### **Physical Chemistry-S-VI (CHE-403P)**

## UNIT- I

Heterogeneous catalysis, Kinetics and mechanism of reactions on surface, Mechanism of surface reactions, Uni and bi-molecular surface reactions, Langmuir-Hinshelwood mechanism, Langmuir-Rideal mechanism, Inhibition of surface reactions, Absolute reaction rate theory of surface reactions.

#### UNIT- II

Comparison of homogeneous and heterogeneous reactions, Study of equilibrium constant and steady state treatment for Arrhenius and Van Hoff's complexes, Influence of substituents on reaction rates (inductive and electromeric effects), Linear free energy relationship, Taft equation, compensation effect, Hammett acidity functions.

#### UNIT- III

a) Oxidation of sugars by  $K_3Fe(CN)_6$  and  $Cu^{+2}$  in alkaline medium, (b) Uncatalyzed and platinum group metals (Osmium, ruthenium, iridium, palladium, rhodium etc.) Catalyzed oxidation of organic and inorganic compounds by  $K_3Fe(CN)_6$  and Ce (IV) etc in acidic / alkaline medium.

#### UNIT- IV

Kinetic of initiation retardation, chain polymerization and ionic polymerization (anionic and cationic), Copolymerisation (with special reference to monomer reactivity ratios).

#### UNIT- V

Coordination polymerization, Degradation of polymers (oxidative, chemical and photolytic), An introduction to conducting polymers, Polyelectrolytes.