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: 2021–2022

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

1. 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 compete 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.

2. 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.

3. 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 prescribed; 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, not shall he/she undertake any remunerative work, though with the prior permission of the Faculty, he/she may join certificate of 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 fours 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, where as 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 **Se**mester 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 Session 2021-2022

The Course of Study and the Scheme of Examinations:

Semester I

Sl. No.	Paper	Code	Type	Title of the paper	Credi	L+T+P	ESE.	IA	Total Mark
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	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	Data generation and interpretation Lab	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 I: One out of three listed below:

CHE104: Solvent Extraction and Chromatography
CHE105: Introduction to Analytical Chemistry I
CHE106: Computer Applications in Chemistry

Note: The Practical Exam shall consist of three papers (each from core papers), each of Six hour's 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	Cre	L+T+P	ESE.	IA	Total Mark
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	Analysis and determination Lab	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 II: One out of three listed below:

CHE204: Forensic Analysis
CHE205: Catalysis and Green Chemistry
CHE206: Introduction to Analytical Chemistry II

Note: The Practical Exam shall consist of three papers (each from core papers), each of Six hour's 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 Mark
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	Hand Made Soap/Detergent Making	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 III: One out of three listed below:

CHE304: Assignment 1 Cheminformatics
CHE305: Assignment 2 Nanochemistry
CHE306: Assignment 3 Green Chemistry

Note: The Practical Exam in each specialization shall consist of three papers (each from core papers), each of Six hour's 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	Credit	L+T+P	ESE.	IA	Total Mark
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-IV		03	2+1+0	45	30	75
6.	Paper-V	CHE407	SD-2	Industrial Laboratory Synthesis	02	2+0+0	30	20	50
7.	Paper-VI	CHE408	UE-2	Nano-chemistr	03	2+1+0	45	30	75
Total					20				500

Elective IV:

CHE404: Research work (Literature survey on any topic concerned with recent developments in chemistry)
CHE405: Industry Visit
CHE406: Field Work

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

Research work/ Industry Visit/Field Work:

Each student has to give a power point presentation on elective paper he/she has chosen. Each presentation will be of 30 minutes duration. Each student has to submit a report based on the topic he/she has chosen which should be consistent with his/her talk. A final examination based on the seminars presented by the students will be conducted at the end of the course. evaluation is done on the basis of oral presentation.

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.

3.4. Paper V (Skill Development) is based on experimental wok. The evaluation of paper V will carried out through laboratory exercises/ practicals including viva-voce and record.

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 Semeste

Syllabus
M.Sc. (Chemistry)
Semester I

Inorganic Chemistry I (CHE-101)

Unit I

Review of Bohr's theory, its limitations and the atomic spectrum of hydrogen atoms. Wave mechanics: de Broglie equation, Heisenberg's Uncertainty Principle and its significance. Schrödinger's wave equation, significance of ψ and ψ^2.Quantum numbers and their significance.Radial and angular wave functions for hydrogen atoms. 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. 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, 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, Werner, Sidgwick and VSEPR theory.

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

Principles of Inorganic Chemistry, B.R.Puri, L.R. Sharma, K.C. Kalia, Milestone Publishers and Distributors/ Vishal Publishing Co.
Advanced Inorganic Chemistry, F.A. Cotton and Wilkinson, John Wiley.
Concise Inorganic Chemistry, J.D. Lee,Wiley.
Inorganic Chemistry, J.E. Huhey, Harper & Row.
Chemistry of the Elements. N.N. Greenwood, A. Earnshow, Pergamon.
Inorganic Electronic Spectroscopy, A.B.P. Lever, Elsevier.
Comprehensive Coordination Chemistry eds., G. Wilkinson, R.D. Gillars and J.A. McCleverty, 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, benzynes and nitrenes.

Unit IV

Aliphatic Nueleophilic Substitution- The S_N2, S_N1, mixed S_N1 and S_N2 and SET mechanisms. The neighboring group mechanism, neighboring 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, ambident nucleophile and regioselectivity.

Unit V

Aliphatic Electrophilic Substitution- Bimolecular mechanisms, - S_E2 and S_E1. The S_E1 mechanism, electrophilic substitution accompanied by double bond shifts. Effect of substrates, leaving group and the solvent polarity on the reactivity.

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

1. Advanced Organic Chemistry, Jagdamba Singh, Pragati Prakashan.
2. Organic Chemistry: Concepts and Applications, Jagdamba Singh, Pragati Prakashan.
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

Brief resume of concepts of laws of thermodynamics, free energy, chemical potential, 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

Linear graphs and slopes, Curve sketching Polynomial, Exponential function, Differentiation formulas, Chain rule, Maxima and minima, Partial and total differential, Exact and inexact differential. Integration, Integration formulas, Permutations and combinations, Probability, Matrices, Determinants, Series, Stirling approximation, Euler reciprocal relation.

Unit III

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 IV

Surface active agents, classification of surface active agents, micellization, hyhrophobic interaction, critical micellar concentration (CMC), factors affectinf the CMC of surfactants, Counter ion binding to micelles, thermodynamics of micellization-phase separation and mass action models, reverse micelles, Micro emulsion.

Unit V

Surface tension, capillary action, Laplace law, Kelvin equation (vapour pressure of droplets), BET equation of estimation of surface area.

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.
3. Physical Chemistry, P.W. Atkins, ELBS.
4. Physical Chemistry, Levine.
5. Thermodynamics, Gurdeep Raj.
6. 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

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-Chlorotoluenefrom p-toluidine.
Cannizzaro reaction: p-Chlorobenzaldehyde as substrate.
Friedel Crafts reaction: Benzoyl propionic acid from succinic anhydride and benzene.
Aromatic electrophilic substitutions: Synihesis of p-bromoanline.
Rearrangement: Synthesis of benzilic acid by benzil-benzilic acid rearrangement. Pinacol-pinacolone rearrangement in Benzpinacol.

Physical Chemistry:

1. Acid base titration using Potentiometry/pH metry.
2. Determine the concentration or percentage of one or two optically active substances in the given solution polarimetrically.
3. Kinetics of oxidation of reducing sugars by potassium ferricyanide/copper(II) in presence of ammonium hydroxide or sodium hydroxide.
4. Kinetics of oxidation of alcohols/diols by aqueous alkaline hexacyanoferrate (III) ions.
5. Conductometric titration of weak/strong acid and strong /weak base.
6. Molecular weight determination using viscometry.

Elective Papers
Solvent Extraction and Chromatography (CHE-104)

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, 2nd 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, 2nd 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.

Introduction to Analytical Chemistry I (CHE-105)

Unit I

Methods of qualitative and quantitative analysis.

Unit II

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

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. Basic Concepts of Analysis Chemistry, S.M. Khopkar, Wiley Eastern.
9. Handbook of Instrumental Techniques for Analytical Chemistry, F. Settle, Prentice Hall.

Computer Application in Chemistry (CHE-106)

Unit I

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,

Unit II

Various types of _I/O'statements, Library functions, Statement functions, Function subprograms and subroutine subprograms.

Unit III

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

Unit IV

Computer programming based on FORTRAN and Numerical methods

Unit V

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]

Skill Development
Data generation and interpretation Lab (CHE-107)

1. Methods of qualitative and Quantitative analysis.

2. Interpretation and statistical analysis of experimental data.

University Elective Paper

Polymer Chemistry (CHE-108)

1. Introduction: Definition and Classification of polymers.

2. Structure, Separation and Properties of Polyethylene, PVC

3. Polymer solutions: Nature, Size and Shapes of Macromolecules in solution.

4. Biomedical and Engineering Application: Tissue engineering, Controlled drug release.

5. Bio polymers DNA, RNA

Books Recommended

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

Semester II
Inorganic Chemistry II (CHE-201)

Unit I

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

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.

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

Advanced Inorganic Chemistry, F.A. Cotton, Wilkinson, John Wiley.
Inorganic Chemistry: Principles of Structure and Reactivity, Huheey, Medhi, Pearson Education India.
Physical Methods in Inorganic Chemistry, R S.Drago, Affiliated East-West Press Pvt. Ltd.
Chemistry of the Elements. N.N. Greenwood, A. Earnshow, Pergamon.
Inorganic Electronic Spectroscopy, A.B.P. Lever, Elsevier.
Comprehensive Coordination Chemistry eds., G. Wilkinson, R.D. Gillars, J.A. Mc Cleverty,Pergamon.

Organic Chemistry II (CHE-202)

Unit I

Aromatic Electrophilic Substitution- The arenium ion mechanism, orientation and reactivity, energy profile diagrams. The ortho/para ratio, ipso attack. Diazonium coupling Vilsmeier reaction, Gatterman-Koch reaction.

Unit II

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 III

Free Radical Reactions- Types of free radical reactions, free radical substitution mechanism, mechanism at an aromatic substrate, neighboring group assistance, reactivity for aliphatic and aromatic substrates at a bridgehead, Reactivity in the attacking radicals. The effect of solvent on reactivity. Allylic halogenation (NBS), oxidation of aldehydes to carboxylic acids, auto oxidation, coupling of alkynes and arylation on aromatic compounds by diazonium salts. Sandmeyer reation. Free radical rearrangement. Hunsdiecker reaction.

Unit IV

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

Unit V

Elimination Reactions- The E_2, E_1 and E_1CB mechanisms, orientation of the double bond. Reactivity-effects of substrate structures, attacking base, the leaving group and the medium. Mechanism and orientation in pyrolytic elimination.

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

1. Advanced Organic Chemistry, Jagdamba Singh, Pragati Prakashan.
2. Organic Chemistry: Concepts and Applications, Jagdamba Singh, Pragati Prakashan.
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.

Unit III

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 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.

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. Physical Chemistry, G. W.Castellan.
4. Statistical Mechanics, B.K. Agarwal, M. Eisner, Wiley Eastern, New Delhi.
5. Statistical Mechanics, R.K. Pathria, Butterworth-Heinemann.
6. Statistical Mechanics, D.A. Mcquarrie, California University Science Books.

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) $VO(acac)_2$

(b) $K_3[Cr(C_2O_4)_3].\ 3H_2O$

(c)) $Na[Cr(NH_3)_2\ (SCN)_4]$

(d) $Mn(acac)_3$

(e) $K_3[Fe(C_2O_4)_3]$

(f)) $Hg[Co(SCN)_4]$

(g) $[Co(Py)_2Cl_2]$

(h) $[Ni(NH)_6]Cl_2$

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 Caffeine from tea leaves
c. Eugenol from cloves

Physical Chemistry: (Any two exercise)

(i) Determination of the velocity constant of the reaction between acetone and iodine catalysed by HCI/H_2SO_4.

(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 pKa 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 Freundilich‘s adsorption isotherm.

(vii) Rast method for determining molar mass.

(viii) Determination of the temperature dependence of E.M.F. using potentiometry/pH metry.

(ix) Determination of the solubility product.

Elective Papers
Forensic Analysis (CHE-204)

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

Instrumentation for Forensic Analysis- 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.

Unit IV

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, 6th Edition (1966), and vol. III B, 5th Edition (1975), Van Nostrand Reinhold Co. London.
2. Peter Fordham, Non-destructive Testing Techniques, 1st edition (1968), London Business Publications Ltd., London
3. W. Horwitz, Official Methods of Analysis, 11th Edition (1970), Association of Official Analytical Chemists, Washington DC.
K. Simpson and B. Knight, Forensic Medicine, 9th Edition (1985), Edward Arnold Publishers Ltd., London.

Catalysis and Green Chemistry (CHE-205)

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.

Introduction to Analytical Chemistry II (CHE-206)

Unit I

Errors analysis: Accuracy and precision, absolute, relative, determinate and indeterminate errors, statistical treatment of random errors, computation rules for significant figures, method of least squares, mean deviations, and standard deviation.

Unit II

Tests of significance, the‘t’ test, the ‘F’ test, the χ^2 (chi-squares) test, distribution normalcy test. Regression analysis; methods of least squares the correlation coefficient, Rejection of observations; the ‘Q’ test.

Unit III

Titrations: Acid-base, complexometric, conductometric and potentiometric titration- theory of acid base indicators, Mohr, Volhard and Fajan’s methods, EDTA based titration, Redox indicators, and their use in volumetric analysis.

Unit IV

Methodology and instrumentation of spectrophotometry in visible, ultraviolet and infra-red regions, spectrometric error, deviation from Beer’s law, analysis of mixtures.
Spectrophotometric methods for investigations of composition and stability of metal complexes in solutions.

Unit V

Separation Techniques: Solvent extraction, thin-layer chromatography, gas chromatography (GC), liquid chromatography (LC), high performance liquid chromatography (HPLC), ion exchange chromatography, gel permeation chromatography. Chromatography coupled instrumentation.

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. Principles of Instrumental analysis, D.A. Skoog, J.L. Loary, W.B. Saunders.
4. Principles of Instrumental Analysis, D.A. Skoog, W.B. Saunders.
5. Quantitative Analysis, R.A. Day, Jr., A.L. Underwood, Prentice Hall.
6. Environmental Solution, S.M. Khopkar, Wiley Eastern.
7. Basic Concepts of Analysis Chemistry, S.M. Khopkar, Wiley Eastern.
8. Handbook of Instrumental Techniques for Analytical Chemistry, F. Settle, Prentice Hall.

Skill Development Paper

Analysis and determination Lab (CHE-207)

1. Analysis of dairy products and petrochemicals.
2. Determination of physico-chemical parameters of waters/ given sample.
3. Food analysis
4. Methods of removal of waste and hazardous metal from water.

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.

University Elective Paper

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

1. Organic chemistry and industry
2. Brief introduction of the molecules Aspirin, adrenaline, coniine, thujone, cholesterol, prostaglandins, penicillines.
3. Overview of antiviral drugs.
4. Bio-polymers: Polysaccharides - starch, cellulose, sucrose
amino acids- polypeptides, proteins.
5. Synthetic polymers: properties and uses - Polyester, poly-tetrafluoroethylene, polyamino acids, polycyanoacrylates, polyurethanes, silicone rubbers, polymeric antioxidants.

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,3rd edition, Pearson Prentice Hall,2005

Specialization Papers
Semester lll
Inorganic Chemistry
Paper-I
Bioinorganic Chemistry -S- l (CHE-301l)

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 phthalocyanines.

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

MetalloProteins and MetalloEnzymes: Function, electronic structure, bonding and stereochemistry of the active site. Natural Oxygen Carrying Proteins-Haemoglobin, Myoglobin, Hemerythrin 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,llW. 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.

Inorganic Chemistry
Paper-III
Organometallic Chemistry of Transition Metals-S- ll (CHE-302I)

Unit I

Inorganic π Acid Ligands: Dioxygen and dinitrogen, nitrosyl, tertiary phosphines and arsines as ligands.Complexes of σ donor ligands: Transition metal alkyls, alkynyls, carbenes and carbines.

Unit II

π 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.

Inorganic Chemistry
Paper-lll
Techniques in Inorganic Chemistry-S- lll (CHE-303l)

Unit I

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

Unit 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.

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

1.E. A. V. Ebsworth, D. W. H. Rankin and S. Cradock, 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, 4thEdn.(1986), John Wiley & Sons, New York.
4.W. Kemp, Organic Spectroscopy, 3rd Edn. (1991), Macmillan, London.
5.G. Aruldhas, Molecular Structure and spectroscopy, Prentice Hall of India Pvt. Ltd., New Delhi

Inorganic Chemistry Laboratory

Separation of a Mixture of Cations/Anions by Paper Chromatographic

technique Using Aqueous/Non-aqueous Media:

a. Pb^{2+} and Ag^{+} (aqueous and non-aqueous media)

b. Co^{2+} and Cu^{2+} (non aqueous media)

c. Cl^{-} and I^{-} (aqueous – acetone media)

d. Br^{-} and I^{-} (aqueous – acetone media)

Ion-exchange Method of Separation

e. Separation of Zn^{2+} and Mg^{2+} on an anion exchanger

f. Separation of Co^{2+} and Ni^{2+} on an anion exchanger

Organic Chemistry
Paper-I

Bioorganic and Medicinal Chemistry-S-1 (CHE-301O)

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 labeling 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 mitoptic 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, hydralaxine, verapamil, methyldopa and diazoxide propanol.

Unit IV

(i) Local Anti-infective Drugs: Antitubercular drugs and Antimalerial 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. B_1, Vit. C_1, Pantothenic acid, Biotin (Vitamin H) and α-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, Pragati Prakashan.
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.

Organic Chemistry
Paper II
Organic Reactions Mechanisms-S-II (CHE-302O)

Unit I

Molecular Rearrangements I:
1. Migration to electron deficient carbon atom - Pinacole-Pinacolone rearrangement, Wagner-Meerweian rearrangement, Tiffenev-Demjanov ring expansion, Dienone-Phenol rearrangement, Benzil-Benzilic acid rearrangement, Favorski rearrangement.

Unit II

Molecular Rearrangements II:
1. Migration to electron deficient nitrogen atom - Wolf, Hofmann, Curtius, Losen, Schmidt, Beckmann rearrangement.
2. Migration to electron deficient oxygen atom - Baeyer-Villiger rearrangement.
3. Stevens, Witting, Neber rearrangements and rearrangement of amino ketones.

Unit III

Oxidation- Introduction, Different oxidative processes. Hydrocarbons-alkenes, aromatic rings, saturated C-H groups (activated and unactivated) Alcohols, diols, aldehydes, ketones, ketals and carboxylic acids, amines, hydrazines, and sulphides. Oxidations with ruthenium tetraoxide, iodobenzene diacetate and thallium. (III) Nitrate.

Unit IV

Reduction- Introduction, Different reductive processes. Alkanes, alkenes, alkynes, and aromatic rings. Carbonyl compounds-aldehydes, ketones, acids and their derivatives. Epoxides - Hydrogenolysis.

Unit V

Organometallic Reagents- Principle, preparations, properties and applications of the following in organic synthesis with mechanistic details. Group I and II metal organic compounds: Li, Mg, Hg, Cd, Zn and Ce Compounds.

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

1. Advanced Organic Chemistry, Jagdamba Singh, Pragati Prakashan.
2. Reactions, Rearrangements and Reagents, S.N. Sanyal, Bharati Bhawan Publishers & Distributors.
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, Comell University Press.
7. Organic Chemistry, R.T. Morrison, R.N. Boyd, Prentice-Hall.
8. Modern Organic Reactions, H.O. House, Benjamin.
9. Organic Reactions and Their Mechanisms, P.S.Kalsi, New Age International,
10. Reaction Mechanism in Organic Chemistry, S.M. Mukherji, S.P. Singh, Macmillan.

Organic Chemistry
Paper III
Organic Photochemistry and Pericyclic Reactions- S-III (CHE-303O)

Unit I

Organic Photochemistry I- Photochemistry of Carbonyl Compounds: Photochemistry of enones, hydrogen abstraction, rearrangements of α, β unsaturated ketones and cyclohexadienones, photochemistry of p-benzoquniones.

Unit II

Organic Photochemistry II- Photochemistry of unsaturated system: Olefins, cis-trans isomerization, dimerization, hydrogen abstraction and additions. Acetylenes-dimerization, Dienes-photochemistry of 1, 3-butadiene, (2+2) additions leading to cage structures, photochemistry of cyclohexadienes.

Unit III

Organic Photochemistry III- Photochemistry of aromatic compounds-exited 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.

Unit IV

Pericyclic Reactions- Molecular orbital symmetry, Frontier orbitals of ethylene, 1, 3-butadiene, 1, 3, 5-hexatriene and allyl system. Classification of pericyclic reactions, Woodward-Hoffmann correlation diagrams. FMO and PMO approach. Electrocyclic reactions-conrotatory and disrotatory motions, 4n, 4n+2 and allyl systems. Cycloadditions-antrafacial and suprafacial additions. 4n and 4n+2 systems, 2+2 addition of ketenes, 1, 3 dipolor cycloadditions and cheleotropic reactions.

Unit V

Sigmatropic rearrangements- Suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon moieties, retention and inversion of configuration, (3,3) and (5,5) sigmatropic rearrangements. detailed treatment of Claisen, Cope and aza-Cope rearrangements. Fluxional tautomerism. Ene reaction.

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

1. Photochemistry and Pericyclic Reactions, Jagdamba Singh,Jaya Singh, New Age International
2. Reaction Mechanism in Organic Chemistry, S. M. Mukherjee, S.P. Singh, Macmillan India Ltd., New Delhi.
3. Pericyclic Reactions, S.M. Mukherjee, S.P. Singh, MacMillan India, New Delhi.
4. Advanced Organic Chemistry / Organic Synthesis, Jagdamba Singh, L D S Yadav, Pragati Prakashan,
5. Pericyclic Reactions, I. Fleming, Oxford University Press, Oxford.
6. Molecular Orbitals and Organic Chemical Reactions, Ian Fleming, Wiley.

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.

(c) Estimation of carbohydrates, protein, amino acids, ascorbic acid, blood cholesterol and aspirin in APC tablets by UV-Visible spectrophotometric method.

Physical Chemistry
Paper –I
Molecular Spectroscopy -S-I(CHE-301P)

Unit I

Molecular Spectra: Basic concepts, classification of spectra, Regions of spectrum
Rotational Spectra: Rigid and non-rigid rotational spectra, selection rule, centrifugal distortion, isotopic shift. Spectra of polyatomic molecules, Inversion and internal roation.

Unit II

Vibration Rotation Spectra: S.H.O., Vibrational energy, Anhormonicity, Rotation- vibration spectra. Selection rule, PQR branches, vibrational spectra of polyatomic molecules.

Unit III

Electronic spectroscopy: Frank-Codon principle, Electronic spectra of polyatomic molecules, Charge -transfer spectra. Quantum theory of Raman spectra, ,Rotational and vibrational Raman Spectra, Resonance Raman spectra, Laser Raman spectra.

Unit IV

NMR spectroscopy: Theory relaxation process and chemical shift. Spin-spin splitting. FT-NMR spectroscopy, 2D NMR spectroscopy, NOE, double resonance, COSY, INDOR, CIDNP.

Unit V

ESR- Principle, g-factor, ESR of anisotropic system, ZFS, ENDOR, ELDOR. Principle of Mossbauer spectroscopy, Origin of line width, Isomer shift, Quadruapole effect.

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).

Joseph R. Lakowicz, Fluorescence Spectroscopy, 2nd edition, Plenum Press, New York. (1999).

Physical Chemistry
Paper –II
Electrochemistry -S-II (CHE-302P)

Unit I

Ionic conductance, Molar conductance, Cell constant, Migration of ions, Transport number and and its determination (Hittorf`s and moving boundary method), Ostwald`s dilution law, Conductometric titration, Potentiometric titration, Grotthus mechanism, Debye-Huckel theory of strong electrolytes, Debye-Huckel-Onsager equation, Wien effect, Debye-Falkenhagen effect.

Unit II

Non-ideal systems: Excess function for non-ideal solutions. Activity, activity coefficient, Debye-Huckel limiting law, Bjerrum`s theory, Application of Phase rule to three component systems, second order phase transition

Unit III

Debye-Huckel theory of activity coefficients, Bjerrum theory of ion association, Dynamic electrochemistry- Electrical double layer, Electrode kinetics, Rate of charge transfer, Current density, Butler- Volmer equation,

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

Fuel cell technology- Fuel cell, Simple Grove's fuel cell, efficiency of fuel cell, SOFC.

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. Physical Chemistry, P.W. Atkins, ELBS.
2. Physical Chemistry, Levine
3. Physical Chemistry, G. W.Castellan.
4. Modern Electrochemistry, Vol. 1, Vol. 2A and Vol. 2 B, J.O'M. Bockris, A.K.N. Reddy,Plenum Press, New York.
5. Electrochemical Methods: Fundamentals and Applications, A.J. Bard, L.R. Faulkner, John Wiley and Sons, New York

Physical Chemistry
Paper –III
Quantum Chemistry -S-III (CHE-303P)

Unit I

Review of classical mechanics. Wave-particle duality and Uncertainty principle. 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 (HCI) 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 Chemistyry, 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. Physical Chemi stry, G. W.Castellan.

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. Conductometry/Potentiometry/pHmetry titration.

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.

Skill Development Paper
Hand Made Soap/Detergent Making (CHE-307)

1. 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.
2. Properties of cleaning agents
3. Technical skill of soap/detergent making
4. Marketing of soap and allied products

University Elective Paper
Environmental Chemistry (CHE-308)

1. **Introduction to Environmental Chemistry:** Concept and scope of environmental chemistry, terminology and nomenclatures, Environmental segments.
2. The natural cycles of environment (Hydrological, Oxygen, Nitrogen)
3. **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.
4. **Air Pollution:** Particulates, Aerosols, SOx, NOx, COx and hydrocarbon, smog, Air-quality standards
5. **Water Pollution:** Water-quality parameters and standards: physical and chemical parameters, Dissolved oxygen, BOD, COD, TDS, 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 Estern Ltd., New Delhi.

Semester IV
Inorganic Chemistry
Paper IV
Spectral Techniques in 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}C NMR; Use of Chemicals as NMR auxiliary reagents (shift reagents and relaxation reagents); 1H NMR of paramagnetic substances.

Unit II

Nuclear Spectroscopy – (ii) Multinuclear NMR of Metal nuclei.^{31}P, ^{9}F, ^{27}Al, ^{11}B, ^{119}Sn.

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 Karamer‘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 AB2, AB3 and AB4 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 Suggested (Names of Publishers may vary as per copyright status):

1.E. A. V. Ebsworth, D. W. H. Rankin and S. Cradock, 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, 4thEdn.(1986), John Wiley & Sons, New York.
4.W. Kemp, Organic Spectroscopy, 3rd Edn. (1991), Macmillan, London.
5.G. Aruldhas, Molecular Structure and spectroscopy, Prentice Hall of India Pvt. Ltd., New Delhi (2001).

Inorganic Chemistry
Paper V
Group theory and Molecular Spectroscopy-S-V (CHE-402I)

Unit I

Group Theory: Introduction, Molecular symmetry and point groups, symmetry elements and operators, classes of symmetry operation, symmetry classification of molecules.Matrix Representation of symmetry operations, representation of groups, character, reducible and irreducible representations, great orthogonality theorem. character tables, symmetry properties of Hamiltonian operator, mutual exclusion principle.

Unit II

Rotational, Vibrational and Electronic spectroscopy: Electromagnetic radiation, interaction of electromagnetic radiation with matter, quantum mechanical approach transition probabilities: Einstein coefficients, pure vibrational and rotational spectra, selection rules, vibrational and rotational spectra of polyatomic molecules, normal modes, an anhorminicity, selection rules.

Unit III

Raman Effect: classical and quantum theory of Raman effect, rotational and vibrational Raman spectra. Franck-Condon principle, transition moments, assignment of electronic transitions of N_2. H_2O and formaldehyde using group theory.

Unit IV

Introduction to NMR: Origin of magnetic moments in matter, electronic and nuclear moments, interaction with magnetic field, Larmor equation - conditions for magnetic resonance absorption, relaxation times, line widths and line shapes, ring currents, diamagnetic anisotropy, spin-spin splitting, high resolution NMR spectra of simple molecules.

Unit V

Other Resonance Spectroscopy Methods:-EPR, NQR and Mossbauer spectroscopic techniques - Electron spin resonance: g value, hyperfine structure, ESR of organic free radicals, ESR of inorganic ions, ESR of simple free radicals in solutions - NQR. The principles of Mossbauer spectroscopy. Origin of isomer shifts, quadrupole splitting and h. f. s.

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

1. Theoretical Inorganic Chemistry by M.C. Day and J. Selbin,
2. Modern Aspects of Inorganic Chemistry by H.J. Emelens and A.G. Sharp.. (Van).
3. Text book of Inorganic Chemistry by P.L. Soni (S. Chand)
4. Inorganic Chemistry by Shriver & Atkins
5. F.A Cotton and G Wilkinson, Advanced Inorganic Chemistry, 6th Edn. (1999), John Wiley & Sons New York.

6 . James E Huheey, Inorganic Chemistry, 4th Edn. (1993) Addison-Wesley Pub. Co, New York.
7. R.S. Drago, Physical Methods in Inorganic Chemistry, International Edn. (1971), Affiliated East-West Press, New Delhi.
8. D.F. Shriver and P.W. Atkins, Inorganic Chemistry, 3rd Edn. (1999), ELBS, London.
9. D.N. Sathyanarayana, Electronic Absorption Spectroscopy and Related Techniques (2001)

Inorganic Chemistry
Paper Vl
Scope of Chemical Biology-S-VI (CHE-403I)

Unit I

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

Unit II

Complexes of Biological Significance: Metal complexes of porphyrins and phthalocyanine, Vitamin B12 and B6; chlorophylls.

Unit III

Metalloproteins: Function, Electronic structure, bonding and stereochemistry of the active site – Natural oxygen carrying proteins – Haemoglobin, Myoglobin, Hemerythrin and Hemocyanin 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 Suggested (Names of Publishers may vary as per copyright status):

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)

Organic Chemistry
Paper-IV
Concepts in Organic Synthesis- S-IV (CHE-401O)

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 regiospecificity: Assymmetric 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 disopropyl amide (LDA). (iv) Dicyclohexylcarbodimide (DCC). (v) 1,3-Dithiane (Reactivity Umpolung). (vi) Trimethylsily 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-Loffler-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, Pragati Prakashan
2. Advanced Organic Chemistry, Jagdamba Singh, Pragati Prakashan.
3. Organic Chemistry: Concepts and Applications, Jagdamba Singh, Pragati Prakashan.
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.

Organic Chemistry
Paper V
Spectroscopic Identification of Organic Compounds S-V (CHE-402O)

Unit I

Introduction to spectroscopic techniques: Electromagnetic spectrum, absorption of energy by organic compounds. Types of spectroscopic methods for organic structure elucidation. Applications of UV – Visible and IR spectroscopies in organic structure elucidation. Various electronic transitions (200-800 nm), Beer-Lambert law. Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ether's, phenols and amines. Detailed study of vibrational frequencies of carbonyl compounds. Effect of hydrogen bonding on vibrational frequencies.

Unit II

Nuclear Magnetic Resonance Spectroscopy- Basic principles. Introduction to NMR techniques. CW and FT NMR techniques. ^{1}H NMR Spectral parameters – intensity, chemical shift, multiplicity, coupling constant. Analysis of first order and second - order spectra. Structure determination of organic compounds by ^{1}H NMR spectra.

Unit III

Carbon-13 NMR Spectroscopy/2-D Spectroscopy- General considerations, chemical shift (aliphatic olefinic , alkyne, aromatic, heteroaromatic and carboynl carbon), coupling constants. Two dimension NMR spectroscopy-COSY, NOESY, DEPT, HMBC and HMQC techniques.

Unit IV

Introduction to mass spectrometry, mass spectral fragmentation of organic compounds, common functional groups, molecular ion peak, metastable peak. Mc Lafferty rearrangement. Nitrogen rule. High resolution mass spectrometry.

Unit V

Solution of Structural problems by joint application of UV, IR, NMR ^{1}H and ^{13}C) and mass spectroscopy.

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

1. Organic Spectroscopy, L.D.S.Yadav, Springer.
2. Elementary Organic Spectroscopy, Y R Sharma, S Chand.
3. Spectroscopy of Organic Compounds, P.S.Kalsi, New Age International.
4. Application of Absorption Spectroscopy of Organic Compounds, J. R. Dyer, Prentice Hall,
   New Delhi.
5. Spectroscopic Identification of Organic Compounds, R.M. Silverstein, F.X. Webster, John Wiley, New York.
6. Spectroscopic Methods in Organic Chemistry, D.H. Williams, I.F. Fleming, Tata-McGraw Hill, New Delhi.
7. Organic Spectroscopy, William Kemp, Palgrave Macmillan.

Organic Chemistry
(Biosynthesis and Chemistry of Natural Products) S-VI (CHE-403O)

Unit I

Bio-synthesis of Natural Products

(a) The acetate hypothesis, poly β-Ketoacids, Biosynthesis, Biogenesis Primary and Secondary reactions involved in biosynthesis. Biosynthesis of poly-ß-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, α terpenol, farnesol, santonin, abietic acid and ß-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'shyadrocarbon 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 PGE2 and PGF2a

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

Physical Chemistry
Paper –I
Spectroscopy and Modern Techniques -S-IV (CHE-401P)

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), EXAFS and SEXAFS.

Unit III

LASER and MASER, NQR spectroscopy,
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.

Unit V

Scanning tunneling and atomic force microscopy (STM and AFM).

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

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

emistry, 1st Edition (1993), Prentice-Hall of India, New Delhi.

Physical Chemistry
Paper –II
Energetics -S-V (CHE-402P)

Unit I

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

Unit II

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

Unit III

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 IV

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 V

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.

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

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

Physical Chemistry
Paper –III
Chemical Dynamics -S-VI (CHE-403P)

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

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 III

Comparison of homogeneous and heterogenous reactions, Study of equilibrium constant and steady state treatment for Arrhenius and Vant 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 IV

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

Unit V

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

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

13. J.M. Hollas, Modern Spectroscopy, 4th edition (2004), John Wiley and Sons, Chichester.
14. C.N. Banwell and E.M. Mc Cash, Fundamentals of Molecular Spectroscopy, 4th edition (1994), Tata McGraw Hill, New Delhi.
15. E.M. Mc Cash, Surface Chemistry, Oxford University Press, Oxford (2001).
16. A.K. Cheetham and P Day, Solid State Chemistry Techniques, Oxford Univ. Press, Oxford (1988).

Joseph R. Lakowicz, Fluorescence Spectroscopy, 2nd edition, Plenum Press, New York. (1999).

Skill Development Paper

Industrial Chemistry Laboratory (CHE-407)

Synthesis of industrially significant chemicals

1. Preparation of alcohol based sanitizer.
2. Synthesis of industrially significant chemicals.

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.