THIRUVALLUVAR UNIVERSITY

SERKKADU, VELLORE - 632 115

DEPARTMENT OF CHEMISTRY

MASTER OF SCIENCE IN CHEMISTRY [Under Choice Based Credit System (CBCS)] **From the academic year 2014-15**

SYLLABUS AND REGULATIONS

FOR UNIVERSITY DEPARTMENT

ABOUT THE DEPARTMENT

The department of chemistry was established 2002 as post-graduate research department. The full fledged department was started during academic year 2010-11. The department is offering the M.Sc., M.Phil. and Ph.D courses. The department consists of 6 faculty members, 2 administrative staff, 37 research scholars and 52 PG students. The faculty members have been working on the modern and thrust areas in chemistry with financial support from various national funding agencies such as DST, DRDO, BRNS, UGC etc., and continued to publish quality research papers in both national and international journals.

VISION AND MISSION

Statement of Vision

The Department of Chemistry of Thiruvalluvar University is determined to educate and graduate rural students. Also, committed to prepare, compete in and contribute to the needs of modern chemical science based industries and academia. To achieve this vision, the department is dedicated to provide a course of study for post-graduate in chemistry which combines curriculum and research oriented project that are high-quality, innovative and intellectually challenging.

Statement of Mission

The mission of the Department of Chemistry of Thiruvalluvar University is to advance the chemical sciences through the education of post-graduate students in rural society by providing them with quality classroom learning and research opportunities. The department is committed to impart a high standard for excellence in all branches of chemistry by innovative and dedicated teaching at post-graduate level to produce students with good knowledge in chemistry.

THIRUVALLUVAR UNIVERSITY
Department of Chemistry
M.Sc., Chemistry (University Department)
UNDER CBCS (With effect from 2014-15)

The course of study and scheme of examinations

1. TITLE: M.Sc., Chemistry.
2. YEAR OF IMPLIMENTATION: June 2014 onwards
3. COURSE DETAILS:

Total No. of Semesters	– 04 (Two semesters per year)
No. of theory papers per semester	– 04
Total No. of theory papers	– 16
No. of practical courses per semester	– 03 (upto 3rd semester)
Total No. of Practicals	– 09
Project	– 4th semester

Total Marks for M.Sc. Degree

Theory	-1600 marks
Practicals	- 900 marks
Project	- 200 marks
Total	**-2700 marks**

4. PREAMBLE OF THE SYLLABUS:

Master of Science (M.Sc.) in Chemistry is a post graduation course of Thiruvalluvar University. The curriculum is prepared by following the prospectus of various national and international universities. The syllabi are all set to meet the standard of UGC-CSIR (NET) and SLET examinations. The credit system to be implemented through this curriculum would allow students to develop a strong footing in the fundamentals and 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 conceptual understanding, development of experimental skills, designing and implementation of novel synthetic methods, developing the aptitude for academic and professional skills, acquiring basic concepts for structural elucidation with hyphenated techniques, understanding the fundamental biological processes and rationale towards computer. The project introduced in the curriculum will motivate the students to pursue the research and find a job in reputed pharmaceutical and other industries including abroad.

5. REQUIREMENT TO APPEAR FOR THE EXAMINATION

(i) Minimum 75% attendance required for both theory and practical examinations.
(ii) Attendance of less than 75% but 65% and above has to pay the condonation fee prescribed by the university.

(iii) Attendance less than 65% but 55% and above has to compensate the shortage of attendance in the subsequent semester (in the next year).
(iv) Attendance less that 55% has to rejoin / redo the semester.
(v) In the case of married woman, the minimum attendance should not be less than 55%.

6. PATTERN OF EXAMINATION

Evaluation of Students:

1. All Semester examinations both theory and practical will be of 100 marks each.
2. Student has to obtain 50% marks in all the examinations (both theory and practicals).

7. FEE STRUCTURE: As per Thiruvalluvar University norms

8. ELGIBILITY FOR ADMISSION

A candidate who has passed the B.Sc., degree examination with Chemistry as the main subject of study of this university or an examination of any other university accepted by the syndicate as equivalent thereto shall be eligible for admission to the M.Sc., degree in chemistry in the university department.

9. MEDIUM OF INSTRUCTION: English.

10. SCHEME OF EXAMINATION

• The semester examination will be conducted at the end of each semester (Both theory & practical examination), for odd semesters in the month of November/December; for even semester in April/May. All theory examination is conducted for 3 hours irrespective of total marks. However, duration of practical examinations is 6 hours.

• **Theory paper** will be of 75 marks each for university examination and 25 marks for internal evaluation.

Theory question pattern

Section-A 10×2 = 20 marks (50 words; no choice)
Section-B 5×5 = 25 marks (200 words; Either or type)
Section-C 3×10 = 30 marks (500 words; 3 out of 5)
Total = 75 marks

Internal Assessment

Test	: 10 marks (best 2 out of 3)
Assignment	: 05 Marks
Seminar	: 10 Marks
Total	**: 25 marks**

There shall be tutorial / practical / surprise test / home assignment / referencing of research papers / seminar / industrial visit / training course as a part of internal assessment in each semester. The students are supposed to

attend all the tests. The students should note that re-test will not be given to the student absent for the test/s.

Practical examination will be of 60 marks each for university examination and 40 marks for internal evaluation.

Distribution of marks for practical examinations

University Examination Experiment : 45 Marks (Procedure 5 marks, Experiment 20 marks, Interpretation 10 marks, Result 10marks)

Practical viva-voce	: 10 marks
Record	: 05 Marks
Total	**: 60 marks**

Practical Internal Assessment

Number of Experiments	: 10 marks
Performance	: 10 Marks
Test	: 20 Marks
Total	**: 40 marks**

Passing Minimum in practical examinations

IA	: 20 Marks (50 %)
UE	: 30 Marks (50 %)
Total	**: 50 Marks**

• For the project report

Report	: 150 marks
Viva-voce	: 50 marks
Total	**: 200 Marks**

Distribution of marks for project report (Total of 150 marks)

Project will be evaluated by the concerned project guide along with a member nominated by the Head of the Department.
Assessment will be done by the departmental committee every month. Evaluation will be on the basis of monthly progress of project work, progress report, referencing, oral, results and documentation.

Project Guide - 100 marks
(Dissertation Format – 20 marks; Scope of the research problem – 20 marks; Methodology – 20 marks; Analysis – 20 marks, Results and findings-20 marks)

Project examiner - 50 marks
(Dissertation Format – 10 marks; Scope of the research problem – 10 marks; Methodology – 10 marks; Analysis – 10 marks, Results and findings-10 marks)

Viva-Voce examination - 50 marks
(Presentation – 20 marks; subject knowledge – 20 marks; Interaction – 10 marks)

11. Question papers will be set in the view of the entire syllabus and preferably covering each unit of the syllabus.

12. STANDARD OF PASSING
A candidate should get not less than 50% in the university examination, compulsorily, in all papers, including practicals. Also, the candidate who secures not less than 50% marks in the UE and IA examinations put together in any theory paper/practical shall be declared to have successfully passed the examination.

Internal marks will not change. Student cannot repeat internal assessment. If student misses internal assessment examination, s/he will have to score passing minimum in the external examinations only.

Illustration: Theory – Internal Assessment -12 marks and University Examination-38 marks

OR

Internal Assessment-0 marks and University Examinaiton-50 marks.

There shall be revaluation of answer script of end semester examination, but not of internal assessment papers.
Internal assessment answer scripts may be shown to the concerned student but not end semester answer script.

- A candidate shall be declared to have passed the whole examination if the candidate passes in all theory and practical by earning 90 credits in core and elective subjects.

13. TRANSITORY PROVISION
This curriculum is valid for three years only, as per UGC norms. Hence, candidates who have undergone M.Sc., Chemistry course in the University department will be permitted to re-appear for next two consecutive years only. After that, he/she has to re-appear for the examinations under new curriculum, regulations, which are in force at that time.

THIRUVALLUVAR UNIVERSITY
DEPARTMENT OF CHEMISTRY
M.Sc., Chemistry (University Department) UNDER CBCS (With effect from 2014-15)
The course of study and scheme of examinations

Subject	Paper Code	General Title	Ins. Hrs./ Week	Cre -dit	Exam hrs	Max. Marks		
						IA	UE	Total
1st Year: I Semester								
Core-1	PDCH 11	Organic Chemistry – I	5	4	3	25	75	100
Core-2	PDCH 12	Inorganic Chemistry - I	5	4	3	25	75	100
Core-3	PDCH 13	Physical Chemistry - I	5	4	3	25	75	100
Elective -1	PDCH 14A	A. Drug Design, Delivery and Action **OR**	3	3	3	25	75	100
	PDCH 14B	B. Modern Separation Techniques **OR**						
	PDCH 14C	C. Chemistry in day to day Context						
Practical-1	PDCH 15	Organic Chemistry Practical - I	4	3	6	40	60	100
Practical-2	PDCH 16	Inorganic Chemistry Practical - I	4	3	6	40	60	100
Practical-3	PDCH 17	Physical Chemistry Practical - I	4	3	6	40	60	100
1st Year: II Semester								
Core-4	PDCH 21	Organic Chemistry – II	4	4	3	25	75	100
Core-5	PDCH 22	Inorganic Chemistry - II	4	4	3	25	75	100
Core-6	PDCH 23	Physical Chemistry - II	4	4	3	25	75	100
Compul -sory	PDHR 20	Human Rights	2	2	3	25	75	100
Elective -2	PDCH 24A	A. Supramolecular and Nano Chemistry **OR**	4	3	3	25	75	100
	PDCH 24B	B. Inorganic Photochemistry **OR**						
	PDCH 24C	C. Materials Chemistry						
Practical-4	PDCH 31	Organic Chemistry Practical – II	4	2	6	40	60	100
Practical-5	PDCH 32	Inorganic Chemistry Practical -II	4	2	6	40	60	100
Practical-6	PDCH 33	Physical Chemistry Practical - II	4	2	6	40	60	100

*IA = Internal Assessment
UE = University Examination

Subject	Paper Code	General Title	Ins. Hrs./ Week	Cre -dit	Exam hrs	Max. Marks		
						IA	UE	Total
2nd Year: III Semester								
Core-7	PDCH 35	Organic Chemistry - III	4	4	3	25	75	100
Core-8	PDCH 36	Inorganic Chemistry - III	4	4	3	25	75	100
Core-9	PDCH 37	Physical Chemistry - III	4	4	3	25	75	100
Elective -3	PDCH 34A	A. Environmental, Green and Sustainable Chemistry **OR**	3	3	3	25	75	100
	PDCH 34B	B. Computational Methods in Chemistry and Chemoinformatics **OR**						
	PDCH 34C	C. Surface Analytical Techniques and Chemical, Electrochemical and Biosensors						
Practical-7	PDCH 35	Organic Chemistry Practical – III	5	3	6	40	60	100
Practical-8	PDCH 36	Inorganic Chemistry Practical - III	5	3	6	40	60	100
Practical-9	PDCH 37	Physical Chemistry Practical – III	5	3	6	40	60	100
2nd Year: IV Semester								
Core-10	PDCH 41	Scientific Research Methodology	3	3	3	25	75	100
Core-11	PDCH 42	Bio-organic and Heterocyclic Chemistry	4	3	3	25	75	100
Elective-4	PDCH 43A	A. Application of Analytical Techniques to Inorganic Compounds **OR**	3	3	3	25	75	100
	PDCH 43B	B. Instrumental Methods of Analysis **OR**						
	PDCH 43C	C. Environmental Chemistry						
Core-12	PDCH 44	Project	20	10	-	50	150	200
		Total	**120**	**90**				**2700**

Core (11 Theory Papers +9 Practicals) : 66 Credits - 2000 marks
Elective (4 Theory Papers) : 12 Credits - 400 marks
Compulsory Paper (Human Rights) : 02 Credits - 100 marks
Project : 10 Credits - 200 marks

Total **: 90 Credits - 2700 marks**

FIRST YEAR: SEMESTER-I

CORE-1 **ORGANIC CHEMISTRY-I**
(Stereochemistry and Reactive Intermediates)

Objectives:

- *On successful completion of the course, the students should have a versatile knowledge of aromaticity and to understood the principles and reaction mechanism involving various electrophilic, nucleophilic, addition.*
- *The course also aims to explain basic concepts in stereo chemistry and conformational analysis of organic molecules.*

Course Out comes: After studying this course the students will be able to:

CO 1. Student should be learning the Aromaticity of aromatic, Antiaromatic and Non-aromatic systems. Then also learn benzenoid and Non benzenoid system.

CO 2. On effective conclusion of the way, the students should have a useful awareness of Stereochemistry, conformational analysisand three dimensional views of the compound it well use full for the unit.

CO 3. Proceeding actual assumption of the way, the students should have a useful awareness of conformational analysis and three dimensional views of the compound it well use full for the unit.

CO 4. On this paper effective end of the progress, the students should must a flexible understanding of reactive intermediates and their study of cationic, anionic, and free radical formation reaction also study in this unit.

CO 5. On prosperous close of the sequence, the students should have a handy acquaintance of Electrophilic, nucleophilic addition reaction and some important naming reaction also study in this unit.

UNIT-I AROMATICITY

Generalization of Aromaticity: Aromaticity of benzenoid and non-benzenoid compounds, Hückel's 4n + 2 Rule, Craig's rule, annulenes; Aromatic and Anti-aromatic Ions-Cations, Anions- Cross-conjugated Systems- Annulenes, Fulvenes and Related Systems. Polycyclic Systems: Cyclopropenyl Aromatic Systems- Pentalenes, Heptalenes, Azulenes - Cyclobutadiene and cyclooctatetraene.

UNIT-II STEREOCHEMISTRY

Newman, Sawhorse and Fisher projection formulae and interconversions; Molecular symmetry and chirality, Classification of Chiral molecules –R-S notation of simple chiral molecules including substituted biphenyls, allenes, helicenes and spiranes, cyclophanes, Re and Si, Pro R and Pro S notations. Illustrations of homotopic, enantiotopic and diastereotopic hydrogen and prochiral carbons with suitable examples. Compounds with two asymmetric carbons - illustrations of *erythro and threo* nomenclature, E Z notations.
Definition with example: Racemic mixture, scalamic mixture, optical purity - enantiomeric excess. Asymmetric synthesis – Cram's rule.

UNIT-III CONFORMATIONAL ANALYSIS

Conformation of simple 1,2 disubstituted ethane derivatives, disubstituted cyclohexanes and halocyclohexane and their stereochemical features, conformations and reactivity of cyclohexanol (acylation and oxidation), reduction of cyclohexanone, esterification and hydrolysis of cyclohexane carboxylic acid derivatives. Sterochemistry of cis and trans decalines, hydrindanes, cyclohexene, cyclooctene, cyclononenes.

UNIT-IV REACTIVE INTERMEDIATES

Carbocations, carbanions, free radicals, radical cations, radical anions, carbenes and nitrenes, arynes – generation, stability, structure and their reactions in C-C bond and other multiple bond formation.

UNIT-V ADDITION REACTIONS

Electrophilic and nucleophilic addition reaction to C=C: Syn and anti additions, Electrophilic addition reactions via halonium & carbocation intermediate, hydroboration, regio- & stereochemistry, electrophilic addition to conjugated dienes, Nucleophilic addition to C=X (X = O, NR): Hydroboration, Michael addition, 1, 3 - dipolar additions including click chemistry, Mannich, Stobbe, Darzen, Wittig, Wittig - Horner and Benzoin reactions. Stereochemical aspects to be studied wherever applicable.

Reference Books

1. Advanced Organic Chemistry part-A. F. A. Carey and R. J. Sundberg, 5th Ed. Springer (2007)
2. Ernest L. Eliel, Stereochemistry of carbon compounds, T.M.H. Edn., Tata McGraw-Hill Publishing Company, 1962.
3. P.S.Kalsi, Stereochemistry – Conformation and Mechanism, New Age International (P) Ltd. 7th Ed., 2008.
4. D.Nasipuri, Stereochemistry of Organic Compounds, New Age International Publishers, 1994.
5. Ernest L. Eliel, Samuel H. Wilen, Sterochemistry of organic compounds, John Wiley & Sons, 2008.
6. Michael B. Smith, Jerry March, March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, John Wiley & Sons, 2007.
7. P.S. Kalsi, Stereochemistry and Mechanism through solved problems, Second Edition, New Age International Publishers, 1994.
8. I. L. Finar, Organic Chemistry, 5th Edn., Vol.2, Stereochemistry and Chemistry of Natural Products, Pearson, 2014.

CORE-2 **INORGANIC CHEMISTRY-I**

(Main Group and Coordination Chemistry)

Objectives:

- *On completion of this course student will have knowledge of Bonding, structure and reactivities of compounds formed by main group elements, and basic knowledge on acid and base concept.*
- *Fundamental theories describe bonding in coordination complexes and structural and other properties such as spectral and magnetic properties of coordination complexes.*

Course Out come:

CO 1. To learn the selected crystal structures and to explain what kind of parameters that affects
CO 2. Understand the basic theories of crystal structure of a compound.
CO 3. Basic knowledge on acid and base concept.
CO 4. Fundamental theories describe bonding in coordination complexes.
CO 5. Understand the structure,stability and reactivity of coordination compound

UNIT-I MAIN GROUP CHEMISTRY-1

VSEPR- dπ-pπ bonding, Bent rule; Allotropes of carbon; Hydrides, Oxides and Oxo acids and nitrides of carbon, nitrogen, oxygen, sulphur, halogens and phosphorous - synthesis, structure, bonding and reactivities. Theories of acid and base. The HSAB concept. Theoretical basis of hardness and softness.

UNIT-II MAIN GROUP CHEMISTRY-2

Strcuture and chemical reactivities of boranes, borazines, S-N compounds, phosphazenes and cyclic phosphazene, silicates and silicones; Interhalogen and Noble gas compounds- Hybridisation, Geometry and properties.

UNIT-III COORDINATION CHEMISTRY-1

Metal-ligand bonding in transition metal complexes- VBT – CFT and CFSE calculation- MOT for octahedral, square planar and tetrahedral complexes. Factors affecting the magnitude of 10 Dq - evidence for crystal field stabilisation- limitations of VBT, CFT - spectrochemical and Nephelauxetic series, site selection in spinels - Jahn-Teller distortion- MOT for sigma and pi bonding in octahedral complexes and- experimental evidence for pi bonding in octahedral complexes.

UNIT-IV COORDINATION CHEMISTRY-2

Terms and states of d_n ions- electronic spectra of coordination compounds - selection rules – Orgel and Tanabe-Sugano diagram for transition metal complexes. Charge transfer spectra. Magnetic properties of coordination compounds - change in magnetic properties of complexes in terms of spin orbit coupling - temperature independent paramagnetism - spin cross over phenomena. The oxidation state, coordination number, stereochemistry, spectral and magnetic properties of Lanthanides and actinides- applications.

UNIT-V COORDINATION CHEMISTRY-3

Structure of coordination compounds - complexes with coordination number one, two, three, four, five and six. - Site preference in trigonal bipyramidal complexes - site preference in square planar complexes - isomerism in five coordinate complexes - Distortion from perfect octahedral symmetry - trigonal prism - geometrical isomerism in octahedral complexes - optical isomerism in octahedral complexes –Cotton effect- absolute configuration of complexes - stereoselectivity and conformation of chelate rings.

Reference Books

1. Inorganic Chemistry - Principles of structure and reactivity, Fourth Edition, J. E. Huheey, E. A. Keiter and R. L. Keiter - Addition Wesley Publishing Co, NY, 1993.
2. Advanced Inorganic Chemistry - F. A. Cotton and G. Wilkinson
3. Mechanism of Inorganic reactions - F. Basolo and R. G. Pear
4. Inorganic Chemistry - R. B. Heslop and P. L. Robinson
5. Introduction to Ligand Fields - B. N. Figgis - Wiley Eastern Ltd, New Delhi, 1976.
6. Inorganic Chemistry- Gary L.Miessler and Donald A. Tarr, person education, Inc
7. Inorganic electronic spectroscopy, A.B.P.Lever, Elsevier.
8. Coordination Chemistry by S F A Kettle, EIBS, 1973.
9. K. F. Purcell and J. C. Kotz, Inorganic Chemistry,-WB Saunders Co., USA, 1977.
10. W. E. Additson, Structural Principle in Inorganic Chemistry, Longman, 1961.
11. A. F. Wells, Structural Inorganic Chemistry, Oxford, V Edition, 1984.
12. Gary Wulfsberz, Inorganic Chemistry.

CORE-3 **PHYSICAL CHEMISTRY-I**

(Thermodynamics and Group Theory)

Objectives:

- *To know the limitations of classical thermodynamics in the evaluation of macroscopic properties.*
- *Learn about the various principles involved in group theory.*
- *To know the knowledge about the construction of character tables.*
- *To know the theories of catalytic activity.*
- *To understand the principles and selection rules for IR and Raman spectroscopy.*
- *To learn about the symmetry of hybrid orbital's.*

Course Out come

CO1. The limitations of calssical thermodynamics in the evaluation of macrocopic properties.
CO2. The varius parinciples invlved in group theory
CO3. The theories of caralytic activity
CO4. The principles and selection rules for IR and Raman spctroscopy.
CO5. The symmetry of hybrid orbitals.

UNIT-I THERMODYNAMICS AND NON-IDEAL SYSTEMS

Second law of thermodynamics-Maxwell relations.

Chemical potential- variation of chemical potential with temperature and pressure, Partial molar quantities-Partial molar volume and partial molar heat content, Van't Hoff isotherm.

Fugacity—Determination of fugacity of gases by graphical method and from equation of state-variation of fugacity with temperature and pressure. Fugacity and mixtures of non-ideal gases-Lewis Randal rule-Duhem-Margules equation. Determination of activity and activity coefficient of non-electrolyte (EMF method)-Ionic strength.

UNIT-II IRREVERSIBLE THERMODYNAMICS

Third law of thermodynamics-Purpose-formulations (Planck, Lewis and Randal)-Thermodynamic properties at absolute zero temperature-calculation of absolute entropies-Apparent exception to third law-Nernst heat theorem.

Thermodynamic criteria for non equilibrium states, generalized flux, forces, matter flow and current flow, entropy production and entropy flow for different irreversible reactions (eg. heat flow, chemical reaction and electrochemical reactions). Non-equilibrium thermodynamics-Basic concepts-Postulates and methodologies-Entropy of irreversible processes-Clausius inequality-Phenomenological equations- Onsager reciprocity relations-Irreversible thermodynamics for biological systems-Coupled reactions.

UNIT-III GROUP THEORY

Basic concepts of groups, Sub-groups-Group Multiplication tables. Abelian and non-Abelian point groups- Representation of cyclic groups.
Symmetry elements and operations – point groups–assignment of point groups to molecules-Matrix representation of geometric transformation and point groups – reducible and irreducible representations–properties of irreducible representation–Similarity transformation-Classes of symmetry operations. Direct product representation-Mulliken's notations and Schoenflies symbols.

UNIT-IV GROUP THEORY AND ITS APPLICATIONS

Great Orthogonality Theorem and its consequences-Construction of character tables for C_{2v}, C_{3v} and D_{2h}.
Applications to molecular vibrations (IR and Raman activity)-Selection rules for IR and Raman spectra-procedure for determining symmetry of normal modes of vibration - Hybrid orbitals in BF_3, CH_4 and NH_3.
Application of group theory for the electronic spectra of ethylene and formaldehyde.

UNIT-V SURFACE CHEMISTRY AND CATALYSIS

Chemisorption and Physisorption; Langmuir's adsorption isotherm; competitive adsorption-Mechanisms of reactions on surfaces (Langmuir-Rideal, Rideal – Eley mechanism and Langmuir-Hinshelwood mechanisms); measurement of surface area, BET equation and Gibb's adsorption. Surface active agent-Classification of surface active agent, Critical Micellar Concentration (CMC), Factor affecting the CMC of surfactants-Microemulsion-Reverse micelles.

Catalysis by enzymes-Rate of enzyme catalysed reactions, effect of pH and temperature on enzyme catalysed reactions-Inhibition. Semiconductor oxides and absorption coefficient and its significance.

Reference Books

1. S. Glasstone, Thermodynamics for chemists, East West Press Pvt. Ltd., New Delhi, 2009.
2. J. Rajaram and J.C. Kuriacose, Thermodynamics for students of chemistry, Pearson, Chennai, 2013.
3. I.M. Koltz and R.M. Rosenberg, Chemical thermodynanics, Benjamin publishers, California, 1972.
4. P.W. Atkins, Physical Chemistry, 7_{th} edn, Oxford University press, 2002.
5. F.A. Cotton, Chemical application of Group theory, 3_{rd} Edition John-Wiley & Sons, Singapore, 2003.
6. K.V. Raman, Group theory and its applications to chemistry, Tata McGraw-Hill, 1994.
7. V. Ramakrishnan and M.S. Gopinathan, Group theory in chemistry, Vishal publications, 1998.

8. Bhattacharya, Group theory and its applications, Himalaya Publishing House, 1992.
9. A.W. Adamson, Physical chemistry of surfaces, 6_{th} Ed., Wiley, 1997.
10. G.A. Somorjai, Introduction to surface chemistry and catalysis, John Wiley, 1994.
11. Maron and Prutton, Principles of physical chemistry, McMillan.
12. W.J. Moore, Physical Chemistry, Orient Longman, London (1972).

ELECTIVE - 1A DRUG DESIGN, DELIVERY AND ACTION

Objectives:

- *Students should be able to understand concepts of drug design and mechanism of drug action of different drugs.*
- *Students will be aware of metabolism and delivery methods of different classes of drugs.*

Course Out come

CO1: Students should be able to understand concepts of drug discovery, drug metabolism and lead Optimization methods. Students will be aware of metabolism and delivery methods of different classes of drugs.
CO2: On successful completion of the paper Students should be able to understand concepts of drug design, and pro drug concepts.
CO3: This unit study for mechanism of drug action of different drugs. The Students should be able to understand concepts
CO4: This unit study for Heterocyclic reaction of fiver member and six membered ring system and also study for the synthesis and proper mechanism
CO5: This unit study for Condensed Heterocyclic reaction of fiver member and six membered ring system and also study for the synthesis and proper mechanism.

UNIT-I DRUG DISCOVERY

An introduction to drugs and receptors, Drug-Receptor interactions, Neurotransmission-Neurotransmitters.
History of drug discovery, Strategies in lead discovery: Ethnopharmaceutical sources, Plant sources, Animal sources, marine sources, drug metabolism studies, observation of side effects.
Lead Optimization methods: Stereochemistry, Bioisosterism, SAR studies.
High throughput Screening.

UNIT-II DRUG DESIGN

Drug design strategies-rational drug design: Inhibitors of ACE; structure based drug design: Anti HIV agents; ligand based approach.

Design of agonist and antagonist: β_2-Agonists and the treatment of asthma, Discovery of the H2–receptor antagonists

Transition state analogues, Pro drug concept: prodrugs of ampicillin, elanapril, propranolol.

UNIT-III DRUG ACTION

Pharmacological activity – Antibiotics: Penicillin; Antimalerials: Trimethoprim; NSAIDS: Paracetamol, Ibuprofen, Diclophenac sodium, Sedatives-Phthalidomide, Hypnotics, Antidepressants: Fluoxetine, Anti-histamines, Anti-tuberclosis agents: Isoniazide , Anti-cancer agents: Vinblastine, Taxol

UNIT-IV DRUG METABOLISM

Adsorption, distribution, metabolism and elimination: Methods of drug administration, drug solubility and lipophlicity, clogP. cell membrane permeability, blood brain barrier Lipinski's rule of five. Metabolism- first pass metabolism, chemical and metabolic stability, bioavailability and bioequivalence, concept of drug half life, therapeutic window.

UNIT - V TYPES OF DRUG DELIVERY SYSTEMS

Types of drug delivery systems, Introduction to Gene Therapy, Types of gene delivery systems, Introduction to targeting, Passive and active targeting, Liposomes, strategies for brain drug delivery, bio distribution, evaluation and applications, time release systems, osmotic systems.

Reference Books

1. Burger's Medicinal Chemistry & Drug discovery, Vol 1-3, 5_{th} Ed, 1995.
2. Chemistry of drug design and drug action-. R. B. Silverman (2004) Acad. press.
3. Graham Patrick, An Introduction to Medicinal Chemistry- 2_{nd} Edn. Qxford, 2010
4. N. K. Jain, Advances in Controlled and Novel Drug Delivery, CBS, 2001.
5. Lednicer, The Organic Chemistry of Drug Synthesis, Vol. 1, 5th Edition, John Wiley & Sons, 2001.
6. Foye's Principles of Medicinal Chemistry, Sixth Edition, Wolters Kluwer, 2008.
7. G.R. Chatwal, Medicinal Chemistry, Himalaya Publishing House.
8. V.K. Ahluwalia and M. Chopra, Medicinal Chemistry, Ane Book Pvt. Ltd., 2008.

ELECTIVE - 1B MODERN SEPARATION TECHNIQUES

Objectives:

- *The students should be able to know the purification and extraction techniques.*
- *This paper enables a student to understand the basic principles of various chromatographic techniques.*
- *The students should be able to understand the advanced microscopic techniques.*

Course Out come

CO1: To gain the Knowledge of synthesis of macromolecules.

CO2: To understand the structure and properties of macromolecules

CO3: To know the liquid crystal polymers of macromolecules

CO4: To understand the preparation and application of industrial polymers

CO5: To study the structure and role DNA and RNA

UNIT-I PURIFICATION TECHNIQUES

Desiccants: types and choice of desiccants, drying of solids. Precipitation: types of precipitation, factors affecting the precipitation. Distillation: theory of distillation. Fractional, steam, azeotropic, vaccum distillations. Recrystallization, Sublimation.

UNIT-II EXTRACTION TECHNIQUES

Solvent extraction: Principle and techniques. Distribution ratio and distribution coefficient. Factors affecting extraction efficiency: Ion association complexes, chelation, synergistic extraction, pH. Numericals based on multiple extractions. Role of chelating ligands, crown ethers, calixarenes and cryptands in solvent extraction. Introduction to Solid phase extraction (SPE) and Microwave assisted extraction (MAE). Applications.

UNIT-III CHROMATOGRAPHY

Definition and Classification. Techniques used in Paper, Thin Layer and Column chromatography. Principle, instrumentation and applications of Gas chromatography(GC), Gas-Liquid chromatography (GLC), High performance liquid chromatography (HPLC), paper electrophoresis. Applications in qualitative and quantitative analysis.

UNIT-IV ION EXCHANGE CHROMATOGRAPHY

Principle and technique. Types of ion exchangers. Ion exchange equilibria. Ion exchange capacity. Effect of complexing ions. Zeolites as ion-exchangers. Applications.

UNIT-V MICROSCOPIC ANALYSES

Scanning Electron Microscopy, Tunneling Electron Microscopy, Scanning Tunneling Microscopy and Atomic Force Microscopy- Principle, Instrumentation and Applications.

Reference Books

1. D.A. Skoog, Principles of Instrumental Analysis, Saunders College Pub.Co, III Edn., 1985
2. A.I Vogel, Text Book of Quantitative Organic Analysis, ELBS III Edn, 1987.
3. D.A. Skoog and D.M. West Fundamentals of Analytical Chemistry, Holt Rinehart and Winston Publications, IV Edn, 2004.
4. Willard, Merit, Dean and Settle, Instrumental Methods of Analysis, CBS Publishers and Distributors, IV Edn.,1989
5. G. D. Christian and J.E.O Reilly, Instrumental Analysis, Allyn and Bacon Inc, II Edn., 1986.

ELECTIVE -1C CHEMISTRY IN DAY TO DAY CONTEXT

Objectives

- *To enable the students to understand the role of chemistry in energy production from renewable resources.*
- *To teach the importance of various types of fuels and their applications.*
- *To create awareness on environmental pollution.*
- *To impart the knowledge on the chemistry of soaps detergents and dyes.*
- *To enable the student to understand chemistry in agriculture.*

Course Out come

CO1: The students should be able to know the purification and extraction techniques.

CO2: To Understand the solvent etraction methods of principle and techniques

CO3: The Students gain the knowledge in paper, thin layer and column chromatography methods

CO4: To know the principle and techniques of Zeolites as ion-exchangers and its applicatios

CO5: The students should be able to understand the advanced microscopic techniques

UNIT-I CHEMISTRY IN ENERGY PRODUCTION

Solar energy – fuel from sun light – splitting of water – hydrogen from sunlight – hydrogen economy - fuel cells - batteries - photovoltaics - stealing the sun - nuclear energy - nuclear fission and fusion - production of electricity by a nuclear reactor - radioactivity and the hazards of radioactivity – living with nuclear power.

UNIT-II ENVIRONMENT

The air we breathe - composition of air - burning of hydrocarbons - fog - air quality -ozone - oxygen/ozone screen - biological effect of UV radiation - ozone formation and distribution in the atmosphere - paths of ozone destruction - chloroflurocarbons and their interactions with ozone – the Antartic ozone hole.

UNIT-III CHEMISTRY OF GLOBAL WARMING

Chemistry of global warming - green house effect - earth's energy balance - vibrating molecules and the green house effect – molecular response to radiation – methane and other green house gases – climate modeling.

UNIT-IV AGRICULTURAL CHEMISTRY

Fertilisers - classification - characteristics and uses - pesticides and insecticides - a brief study of additives use and abuse of additives in foods and beverages.

UNIT-V DYES, SOAPS AND DETERGENTS

Dyes - classification based on mode of application and structure - paints - ingredients -drying – pigments – types and properties – varnish. Soaps and detergents - classification - ingredients - solids and liquids - disinfectants (phenyl, dettol type) - perfumes - raw materials - perfumes used in soaps - cosmetics and agarbatti.

Reference Books

1. B.K.Sharma, Industrial Chemistry (Including Chemical Engineering), (10 Th Edition),
2. M.Gopala Rao, Outlines of Chemical Technology – For the 21_{st} Century – & Marshall Sittig, 3 rd Edition.
3. Bailey, Clark, Ferris, Isrause, Strong, Chemistry of the environment, 2_{nd} Edn, 2001, Elsevier publications.
4. Energy resources and the environment, V. K. Prabhakar, 2001.
5. Fundamental Concepts of Applied Chemistry, Jayashree Ghosh, S.Chand, 2005

PRACTICAL-1

ORGANIC CHEMISTRY PRACTICAL - I

Course Objectives

- Identification of components in a two component mixture and preparation of their derivatives- Any six binary mixtures.
- Determination of m.p. of solid compounds/derivatives.

Course Out come

CO 1: To familiarize the systematic producers organic substances analysis

CO2: To learn two stage preparation involving molecular rearrangement oxidation .

CO3: To know the preparation involving nitration and bromination.

CO4: To familiarize the test involving identification of special elements

CO5: To learn the confirmatory test for various functional groups.

1. Identification of components in a two component mixture and preparation of their derivatives- Any six binary mixtures.
2. Determination of m.p. of solid compounds or derivatives.

Reference Books

1. Arthur I. Vogel, "A Textbook of Practical Organic Chemistry", ELBS.
2. N.S. Gnanapragasam and B. Ramamoorthy, "Organic Chemistry Lab Manual" (2006), S. Visvanathan Printers & Publishers.
3. Raj K. Bansal, Laboratory Manual of Organic Chemistry, Wiley Eastern Limited.
4. Mann and Saunders, Laboratory manual of Organic Chemistry.

PRACTICAL-2

INORGANIC CHEMISTRY PRACTICAL - I

Course Objectives

- To understand the analysis of inorganic mixture and find out the four radicals.

Course Out come

CO1: To Know the Qualitative analysis of inorganic mixture.
CO2: Analysis of the vaious inorganic mixture of compounds.
CO3: Understand the procedure to determine the rare earth elements.
CO4: Know the separation techniques of rare earth elements.
CO5: To get knowledge of Separation of inorganic elements.

Semi micro qualitative analysis of inorganic mixture containing two common and two rare earth cautions.

The following are the rare earth cations to be identified.

W, Se, Te, Mo, Ce, Th, Ti, Zr, V, Be, U, Li.

Reference Books

1. J.Mendham, R.C.Denney, J D Barnes, M. Thomas and B. Sivasankar, Vogel's text book of quantitative chemical analysis, Pearson Educaion Ltd., Indian subcontinent edition, 2009.
2. V.V. Ramanujam, "Inorganic Semi Micro Qualitative Analysis", 3rd Edn. The National Publishing Company (1994 reprint 2004)

PRACTICAL-3

PHYSICAL CHEMISTRY PRACTICAL - I

Course Objectives

- To understand the acid hydrolysis and iodination of acetone.

Course Out come

CO1: Acid Hydrolysis of ester
CO2: Kineticss of iodination of acetone
CO3: Study of Association of Benzoic acid in Benzene
CO4: Study of phase diagram of two components froming simple eutectic.
CO5: Study of the salt effect on the reaction between acetone and iodine.

1. Kinetics – Acid Hydrolysis of Ester – Comparison of strengths of acids.
2. Kinetics – Acid Hydrolysis of Ester – Determination of Arrhenius parameters.
3. Kinetics – Persulphate – Iodide Reaction – Determination of order, effect of Ionic strength on rate constant.
4. Kinetics of saponification of ester.
5. Primary salt effect (Clock reaction) for the reaction between persulphate and iodide.
6. Kinetics of iodination of acetone.
7. Distribution Law – Study of Association of Benzoic Acid in Benzene.
8. Adsorption –Oxalic Acid\Acetic Acid on charcoal using Freundlich isotherm.
7. Study of phase diagram of two components forming simple eutectic.
8. Study of inversion of cane sugar in the presence of acid using polarimeter.
9. Study the salt effect on the reaction between acetone and iodine.
10. Determination of molecular weight by Rast method.
11. Study of the equilibrium constant of the reaction between KI and I_2.
12. Distribution of acetic acid between water and chloroform.

Reference Books

1. Practical Physical Chemistry by B. Viswanathan and P.S. Raghavan, Viva publishers.
2. Findlay`s practical Physical Chemistry , `Revised and edited by B.P. Levitt, 9th edn., Longman, London, 1985.
3. J.N,Gurtur and R.Kapoor,"Advanced Experiemental Chemistry," Vol.I, S.Chand & Co., Ltd., New Delhi.

SEMESTER-II

CORE-4 **ORGANIC CHEMISTRY-II**
(Organic Reaction Mechanisms and Rearrangements)
Paper Code: TUCH21

Objectives:

- *This paper explains the basic concepts of substitution reaction and elimination reaction. Mechanism of some of the important rearrangements in organic chemistry will be discussed.*

In addition the students will gain knowledge on reaction mechanism and synthetic application of oxidation and reduction reactions in organic synthesis.

Course Out come

CO1: This unit explicates the plain theories of substitution Oxidation and reduction reactions in organic synthesis. In calculation the students will advantage information on reaction mechanism.

CO2: This paper explains the basic concepts of substitution reaction and Synthesis techniques of the active group. In addition the students will gain knowledge on reaction mechanism.

CO3: This paper explains the basic concepts of Elimination reaction andSynthesis techniques of sum elimination reactions. In addition the students will gain knowledge on reaction mechanism.

CO4: This red-top describes the elementary concepts of molecular rearrangements reaction in organic chemistry will be discussed. In count the students will advance understanding on reaction mechanism.

CO5: This broadside explains the basic concepts of s naming reaction and reagents in organic synthesis. In addition the students will gain knowledge on reaction mechanism and synthetic application.

UNIT-I SUBSTITUTION REACTIONS

Aliphatic Substitution Reactions: Mechanism of aliphatic substitution reactions -S_N1, S_N2, S_Ni, mechanism– non-classical carbocations-Neighboring group participation. Substitution at carbonyl, vinylic and bridgehead systems – substitution by ambident nucleophiles- HVZ reaction, Stark-Enamine reaction. Aliphatic electrophilic substitution: SE1, SE2 and SEi mechanism. Aromatic Substitutions: Electrophilic substitution-the arenium ion mechanism. Orientation and reactivity (ortho, meta and para directing groups). Typical reactions including Vilsmeyer - Haack, Schilmann reaction-Synthesis of di and trisubstituted benzene (symmetrical tribromo benzene, 2-amino-5-methylphenol, 3-nitro-4-bromobenzoic acid, 3,4-dibromonitrobenzene) starting from benzene. Nucleophilic substitution - methods for the generation of benzyne intermediate and reactions. Chichibabin reaction.

UNIT-II ELIMINATION REACTIONS

E1, E2 and E1CB mechanism - E1, E2 and E1cB spectrum - Orientation of the double bond -Hoffman and Saytzeff rules - Competition between elimination and substitution. Chugaev and Cope eliminations. Typical eliminations reactions - dehydration, dehydrohalogenation and dehalogenation. Stereochemistry of E2 eliminations in cyclohexane systems. Mechanism of pyrolytic eliminations.

UNIT-III OXIDATION AND REDUCTION REACTIONS

Oxidation: Carbon Oxidation Number -Calculation. Study of the following oxidation reactions: chromium trioxide, Osmium tetraoxide, DDQ, Chloranil-Alkenes to epoxides and dihydroxy compounds; Oxidation of alcohols using PCC, PDC, Jones, Dess-Martin oxidation; Sharpless epoxidation, Oppenauer oxidation, Oxidation using DMSO, $KMnO_4$, $Pb(OAc)_4$, SeO_2, Ozonolysis.

Reduction: Selectivity in reduction of 4-t-butylcyclohexanone using selecterides. Hydride reductions - reduction with $LiAlH_4$, $NaBH_4$, tritertiarybutyloxyaluminium hydride, sodium Cyanoborohydride, trialkyltin hydride, hydrazines. MPV reduction, Birch reduction, Asymmetric reduction-Itsuno, Corey and Nyori.

UNIT-IV MOLECULAR REARRANGEMENTS

A detailed study with suitable examples of the mechanism of the following rearrangements: Wagner - Meerwein, Demjanov, Dienone - phenol, Favorski, Baeyer - Villiger, Wolf, Stevens (in cyclic systems) Sommlet Hauser and Von Richter rearrangements.

UNIT-V NAMED REACTIONS AND REAGENTS IN ORGANIC SYNTHESIS

Reagents: Lithium dialkyl cuprates, lithium diisopropylamide(LDA), Dicyclohexylcarbodiimide(DCC), Trimethyl silyl iodide. Named Reactions: Mannich reaction, Biginelli Reaction, Henry reaction, Perkin reaction, McMurry coupling, Robinson annulation, Bischler–Napieralski reaction, Buchwald–Hartwig amination, Baylis-Hilmann reaction. Pd catalysed coupling reactions: Stille, Negishi, Heck, Suzuki, Glazer-Ellington coupling. Miyamura, Barton and Shapiro reaction, Hoffmann-Loffler-Freytag reactions.

Reference Books

1. R.T. Morrison, R.N. Boyd, Bhattacharjee, Organic Chemistry, seventh edition, Pearson, 2014.
2. S.H.Pine, J.B. Hendrickson, D.J.Cram and G.S.Hammond, Organic Chemistry, IV Edn., McGraw-Hill Company 1980.
3. P.S.Kalsi, Organic Reactions and Mechanisms, II Edn. New Age International Publishers, 2000.
4. J.M.Harris and C.C. Wamser, Fundamentals of Organic Reaction Mechanisms, John Wiley & Sons, Inc. 1976.
5. Jonathan Clayden, Nick Greeves, Stuart Warren, Organic Chemistry, second edition, Oxford University press, 2012.
6. E.S. Gould, MechanismandStructures in Organic Chemistry, Holt, New York (1959).
7. Mc Murry,Organic Chemistry,V Edition, Asian Books Pvt Ltd (2000).
8. R.O.C. Norman, Organic Synthesis, Chapman and Hall, NY(1980).
9. S.M. Mukherji and S.P. Singh, Organic Reaction Mechanism, MacMillan India Ltd., Chennai (1990).
10. T.L. Gilchrist and C.W. Rees, Carbenes, Nitrenes and Arynes, Thomas Nelson and Sons Ltd., London.
11. Peter Sykes, A Guide book to mechanism in organic chemistry, Pearson Edn., (2006).

CORE- 5 **INORGANIC CHEMISTRY-II**

(Coordination and Organometallic Chemistry)

Objectives:

- *On completion of the course the students will have the knowledge of fundamental mechanism of reactions of coordination complexes*
- *Basic concepts of bonding in organometallic chemistry, and synthesis, structure, reactivity and uses of different organometallic complexes.*

Course Out come

CO1: Basic concepts and functions of Bio-Inorganic complexes.
CO2: Understand the Mechanism of various biological reaction in Bio inorganic Chemistry
CO3: Know the mechanisms of Organic metallic compounds in Bio inorganic complexes.
CO4: Basic concepts of bonding and catalysis in organic metallic compounds.
CO5: Understand the Concept of Organic metallic Compounds.

UNIT-I COORDINATION REACTIONS

Substitution reactions in square planar complexes – Trans effect- Theories of trans effect – Reaction mechanism and kinectics of nucleophilic substitution in octahedral complexes - reaction rates influenced by acid and bases - racemisation and isomerisation - mechanisms of redox reactions - outer sphere mechanisms - excited state outer sphere electron transfer reactions - inner sphere mechanisms –Marcus-Hush theory- mixed valent complexes.

UNIT-II ORGANOMETALLICS-1

Definition of organometallic compound - 18 electron rule - EAN rule - classification of organometallic compounds - the metal carbon bond types - ionic bond - sigma covalent bond - electron deficient bond - delocalised bond - dative bond-Metal carbonyl complexes – preparation, structure, reactivities and vibrational spectra of metal carbonyls- metal carbonyl clusters - Wades rule and isolobal relationship - metal nitrosyls - dinitrogen complexes - dioxygen complexes.

UNIT-III ORGANOMETALLICS-2

Metal alkyl complexes - stability and structure - synthesis by alkylation of metal halides - by oxidative addition - by nucleophilic attack on coordinated ligands - metal alkyl and 18 electron rule - reactivity of metal alkyls - M-C bond cleavage reactions - insertion of CO to M-C bonds - double carbonylation - insertions of alkenes and alkynes - insertions of metals with C-H bonds- Pi-complexes with unsaturated molecules- alkene, alkyne, allyl, dienyl and trienyl complexes-preparation, bonding and structure and applications.

UNIT-IV METALLOCENES

Cyclopentadienyl complexes - metallocenes – synthesis, bonding and reactions- -bent sandwich complexes - bonding in bent sandwich complexes - metallocene halides and hydrides - metallocene and stereospecific polymerisation of 1-alkenes - cyclopentadiene as a non-spectator ligand - Half-sandwich complexes

-synthesis and structures of allyl complexes -arene complexes - synthesis - structure and reactivity of arene complexes - multidecker complexes.

UNIT-V ORGANOMETALLIC CATALYSTS

Organometallic compounds in homogeneous catalytic reactions - coordinative unsaturation - acid-base behaviour reaction - migration of atoms or groups from metal to ligand - insertion reaction - reactions of coordinated ligands - catalytic reactions of alkenes - isomerisation of alkenes-hydrogenation– hydroformylation-wacker process- Wilkinson catalyst- hydrosilation of alkenes - alkene polymerisation and oligomerisation- Zeigler-Nata catalyst - fluxional molecules.

Reference Books

1. Organometallics 1, complexes with transition metal-carbon -bonds, Bockmann, Oxford science publications, Oxford, 1996.
2. Organometallics 2, complexes with transition metal-carbon -bonds, Bockmann, Oxford science publications, Oxford, 1996.
3. Basic organometallic chemistry, J. Haiduc and J. J. Zuckerman, Walter de Gruyter, Brelin, 1985.
4. Inorganic Chemistry - Priciples of structure and reactivity, J. E. Huheey Harper International Edition, Harper and Rone New York, 1978.
5. Advanced Inorganic Chemistry, F. A. Cotton and G. Wilkinson, Fourth Edition.
6. Inorganic Chemistry- Gary L. Miessler and Donald A. Tarr, pearson education, Inc

CORE-6 **PHYSICAL CHEMISTRY-II**

(Chemical Kinetics and Quantum Chemistry)

Objectives:

- *To elucidate the use of chemical kinetics in understanding react ion mechanisms and to apply the theories and concepts of it for homogenous and heterogeneous catalysed reactions.*
- *To understand and appreciate the quantum mechanical approach to the atomic and molecular electronic structure.*
- *To become familiar with the required mathematics for solving quantum mechanical problems.*
- *To know the limitations of quantum chemistry and classical thermodynamics in the evaluation of macroscopic properties.*
- *To understand the inter linking of quantum chemistry and statistical thermodynamics that leads to classical thermodynamics.*
- *To apply the concepts of statistical thermodynamics for the study of equilibrium reactions and reaction rates.*

Course Out come:

CO1: The use of chemical kinetics in understanding reaction mechanism and to apply the theories and concepts of it for homogenous and heterogeneous catalysed reactions.
CO2: The quantum mechanical approach to the atomic and molecular electronic structure.
CO3: The required mathematics for solving quamtum mechanical problems.
CO4: The limatations of quantum chemistry and classical thermodynamics in the evaluation of macroscopic properties.
CO5: The concepts of statistical thermodynamics for the study of equilibrium reactions and reaction rates.

UNIT-I CHEMICAL KINETICS-I

Collision theory of reaction rates-Steric factor-Lindemann's theory.
Probability factor- potential energy surfaces and contour diagrams- Principle of microscopic reversibility - Steady–state approximation- Theory of absolute reaction rates-Comparison of transition state theory with collision theory-Eyring equation-Thermodynamic and partition function approaches-significance of entropy and enthalpy of activation-linear free energy relationships-Hammett and Taft equations-kinetic isotopic effect- Partition function and activated complex.

UNIT-II CHEMICAL KINETICS-II

Application of ARRT to solution kinetics - influence of solvent, ionic strength, dielectric constant and pressure on rates in solution - Rate expressions for opposing, parallel and consecutive reactions; Chain reactions-Rice-Herzfield mechanism.Explosions.
Acid-Base catalysis-Mechanism-Bronsted catalysis law-Skrabal diagram-prototropic and protolytic mechanisms-acidity function.
Fast reactions-Laser Flash photolysis, flow technique and relaxation methods.

UNIT-III QUANTUM CHEMISTRY-I

Inadequacy of classical mechanics, Black body radiation, Planck's radiation law-Photoelectric effect-Compton effect- Bohr's theory of hydrogen atom-Hydrogen spectra, Wave-particle dualism, Uncertainty principle-Schrödinger equation-1D and 3D, Postulates of quantum mechanics.
Operators: Algebra operator, commutation operator, linear and hermitian operator, eigen functions and eigen values, angular momentum operator.
Applications of Schrödinger equation to simple systems—particle in a box, one and three-dimensional-Orthogonalisation and normalisation-QM tunneling.

UNIT-IV QUANTUM CHEMISTRY-II

Applications of wave mechanics- Rigid rotator, Harmonic oscillator – Hydrogen atom solution-Origin of quantum mechanics.
Approximation methods—Variation methods, Perturbation method for non-degenerate systems-Slater determinant-Anti-symmetric wave functions-Application to Helium atom-Born-Oppenheimer approximation.
Spin orbit interaction, L-S and j-j coupling schemes—Hartree-Fock SCF method for many electron systems. Application of HMO treatment to ethylene, butadiene and benzene.

UNIT-V STATISTICAL THERMODYNAMICS

Classical statistics-Maxwell-Boltzmann (MB) statistics-Phase space-Sterling approximation-Derivation of distribution function-Contradiction of MB statistics with Heisenberg uncertainty principle. Other forms of MB distribution function.
Quantum statistics-Bose-Einstein (BE) and Fermi-Dirac (FD) statistics-Derivation of distribution function-MB, BE and FD statistics comparison-Partition function-Translational and rotational partition function (Problem only)-Ortho and para hydrogen.

Debye and Einstein heat capacity of solids-Assumptions-Merits and limitations. Negative Kelvin temperature.

Reference Books

1. K.J. Laidler, Chemical Kinetics, Pearson, 5th edition, 2011.
2. J. Rajaram and J.C. Kuriacose, Kinetics and Mechanisms of chemical transformations: Application to Femtochemistry, McMillan, 2011.
3. Agarwal, Basic chemical kinetics, Tata McGraw-Hill, 1990.
4. R.G. Frost and Pearson, Kinetics and mechanism, Wiley, New York.
5. Gordon M.Barrow-Physical Chemistry,Mc Graw Hill Publishing Company Ltd., 2007.
6. R.K. Prasad, Quantum chemistry, Wiley Eastern, 1993.
7. W. Levine, Quantum chemistry, Prentice-Hall, 2000.
8. D.A. McQuarrie, Quantum chemistry, University science books, MilValley, California, 1998.
9. P.W. Atkins, Molecular Quantum mechanics, Clarendon Press New York, 2009.
10. R. Anantharaman, Fundamentals of Quantum chemistry, McMillan India.

11. Thomas Engel and Philip Reid, Quantum Chemistry and Spectroscopy , Pearson, 6th edition, 2012.
12. A. K. Chandra, Introductory quantum chemistry, 4th ed,. Tata McGraw Hill 1994.
13. H.K. Moudgil, Text Book of Physical Chemistry, PHI Learning, New Delhi, 2010.
14. Thomas Engel and Philip Reid, Thermodynamics: Statistical thermodynamics and Kinetics, Pearson, 2012.
15. M.C. Gupta, Statistical thermodynamics, New Age International, Pvt., Ltd., New Delhi, 1995.
16. F.W. Sears, G.L. Salingar Turcotte; Statistical thermodynamics, Narosa Publishing house New Delhi, 1998.
17. R. Hasee, Thermodynamics of Irreversible Process, Addition Wesley, Reading.
18. Thomas Engel and Philip Reid, Physical Chemistry, Third Edition, Pearson, 2014.

COMPULSORY PAPER

HUMAN RIGHTS

Course Objectives

- To understand historical development and theories- international human rights.

Course Out comes

CO1: Apply effective written and oral communication skills to business and legal situations.
CO2: Analyze the global legal environment
CO3: Students will graduate with the ability to analyze complex problems, find and deploy a variety of legal authorities, and communicate effectively in a variety of settings
CO4: Use critical thinking skills in business situations.
CO5: Apply an ethical understanding and perspective to business situations.

UNIT-I HISTORICAL DEVELOPMENT AND THEORIES

Definition of Human Rights - Nature, Content, Legitimacy and Priority - Theories on Human Rights - Historical Development of Human Rights.

UNIT-II INTERNATIONAL HUMAN RIGHTS-1

Prescription and Enforcement up to World War II - Human Rights and the UNO-Universal Declaration of Human Rights - International Covenant on Civil and Political Rights - International Covenant on Economic, Social and Cultural Rights and Optional Protocol.

UNIT-III HUMAN RIGHTS DECLARATIONS

U.N. Human Rights Declarations - U.N. Human Commissioner.

UNIT-IV INTERNATIONAL HUMAN RIGHTS-2

Amnesty International - Human Rights and Helsinki Process – Regional Developments - European Human Rights System - African Human Rights System - International Human Rights in Domestic courts.

UNIT-V HUMAN RIGHTS FOR CHILDREN AND WOMEN

Contemporary Issues on Human Rights: Children's Rights - Women's Rights - Dalit's Rights - Bonded Labour and Wages - Refugees - Capital Punishment. Fundamental Rights in the Indian Constitution - Directive Principles of State Policy - Fundamental Duties - National Human Rights Commission.

Reference Books

1. International Bill of Human Rights, Amnesty International Publication, 1988.
2. Human Rights, Questions and Answers, UNESCO, 1982
3. Mausice Cranston - What is Human Rights
4. Desai, A.R. - Violation of Democratic Rights in India

6. Timm. R.W. - Working for Justice and Human Rights.
7. Human Rights, A Selected Bibliography, USIS.
8. J.C.Johari - Human Rights and New World Order.

10. Amnesty International, Human Rights in India.
11. P.C.Sinha-International Encyclopedia of Peace, Security
12. K. Cheous (Ed) Social Justice and Human Rights (Vols 1-7).
13. Devasia, V.V. - Human Rights and Victimology.

Magazines:

1. The Lawyer, Bombay
2. Human Rights Today, Columbia University
3. International Instruments of Human Rights, UN Publication
4. Human Rights Quarterly, John Hopkins University, U.S.A.

ELECTIVE-2A SUPRAMOLECULAR AND NANO CHEMISTRY

Objectives:

- *On completion of the course the student should know the basis of suprmolecular chemistry, metal-organic framework solids, nano mateirlas and their applications.*
- *Various techniques available to characterize the advanced Inorganic materials*

Course Out comes

CO1: To know the basis of supramolecular Chemistry, meat-organic framework solids,nanomaterials and their applications.
CO2: Various techniques available to characterize the advanced inorganic materials.
CO3: To know the basic concepts of nano chemistry of materials.
CO4: Understand the various techniques of preparation of nano materials.
CO5: Explore the theoretical understanding of various physical and chemical properties of nanomaterials.

UNIT-I SUPRAMOLECULAR CHEMISTRY

Introduction to supramolecular chemistry- Definitions and classification of non-covalent interactions- supramolecular synthons-Molecular recognition-self assembly- Supramolecular chemistry of metal containing compounds-1D, 2D, 3D- Host-Guest compounds-Alpha-, Beta-, Gamma-cyclodextrins..

UNIT-II FRAMEWORK SOLIDS

Introduction-definition of porosity, pore size, pore volume, pore density-zeolites-synthesis and applications-metal organic frame work solids-definition-classifications- uses of different types of organic ligands- tuning of structure and properties - synthetic methods- Advantage of MOF solids over zeolites-cracking of petroleum products

UNIT-III NANOCHEMISTRY

General introduction to nanomaterials and emergence of nanotechnology; Synthesis of nanoparticles of ZnO_2, TiO_2, silver, gold, rhodium, palladium, platinum, and; carbon materials- fullerene- porous nano carbon(PNC)-synthesis

Techniques of synthesis: electroplating and electro-phoretic deposition, conversion through chemicalreactions and lithography; Thin films:Chemical vapor deposition and Atomic layer deposition techniques; Carbon fullerenes and nanotubes.

UNIT-IV ANALYTICAL TECHNIQUES

Electronic microscopes- SEM – TEM - X-ray diffraction-EXAFS - Nitrogen adsorption-desrption method-TG/DTA/DSC methods-instrumentation and interpretations and applications.

UNIT-V ADVANCED INORGANIC MATERIALS

Applications of Advanced Inorganic materials in catalysis-gas adsorption-gas storage-sensors.

Reference Books

1. Supramolecular chemistry, J.M.Lehn, VCH
2. C.N.R. Rao, A. Muller, A.K. Cheetam (Eds), The Chemistry of Nanomaterials, Vol.1, 2, Wiley – VCH, Weinheim, 2004
3. Nanochemistry, Kenneth J. Klabunde and G.B.Sergeev
4. G.Zhong Cao. Nanostructures and Nanomaterials: Synthesis, Properties and Applications, Imperial College Press (2004)
5. Metal-Organic Frameworks Applications from Catalysis to Gas Storage. Cejka, J, ed. (2011). Wiley-VCH. ISBN 978-3-527-32870-3
6. Zeolites and Catalysis: Synthesis, Reactions and Applications. Jiri Cejka; Avelino Corma; Stacey Zones (2010). John Wiley & Sons. ISBN 978-3-527-63030-1.

ELECTIVE-2B

INORGANIC PHOTOCHEMISTRY

Objectives:

- *On the completion of the course the student will have the knowledge of basic principle of inorganic photochemistry*
- *Instrumentation techniques used in Inorganic photochemistry*
- *Application of photochemical properties such as sensitizer of Inorganic compounds.*

Course Out comes

CO1: The students will have the knowledge of basic principle of inorganic photochemistry
CO2: To understand the concept of excited states of metal complexes
CO3: To know the instrumentation techniques used in inorganic photochemistry
CO4: To study the energy transfer under conditions of weak and strong interaction in redox reaction.
CO5: To know the application of photochemical properties such as sensitizer of inorganic compounds

UNIT-I PHOTOPHYSICAL PROCESSES

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

UNIT-II METAL COMPLEXES

Excited states of metal complexes: Comparison with organic compounds, electronically excited states of metal complexes, charge transfer spectra, charge transfer excitations.

UNIT-III PHOTOREACTIONS

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

UNIT-IV REDOX REACTIONS

Energy transfer under conditions of weak interaction and strong interaction-examples formation; condition of the excited states to be useful as redox reactants, excited electron transfer, metal complexes as attractive condidates, (2,2-bipyridine and 1,10-phenanthroline complexes), illustration of reducing and oxidising character of $[Ru(bipy)_3]_{2+}$ complex, comparsion with $[Fe(bipy)_3]_{2+}$;role of spin-orbit coupling-life time of these complexes. Application of redox processes of electronically excited states for catalytic purposes, transformation of low energy reactants into high energy products, chemical energy into light.

UNIT-V APPLICATIONS

Metal complex sensitizer, electron relay, metal colloid systems, semiconductor supported metal or oxide systems, water photolysis, nitrogen fixation and carbon dioxide reduction.

Reference Books:

1. Concepts of Inorganic Photochemistry, A.W. Adamson and P.D. Fleischauer, Wiley.
2. Inorganic Photochemistry, J.Chem. Educ. vol. 60 No. 10, 1983.
3. Progress in Inorganic Chemistry, Vol. 30ed. S.J. Lippard. Wiley. Coordination Chem. Revs. 1981, vol. 39, 121, 1231, 1975, 14, 321,; 1990 97, 313.
4. Photochemistry of Coordination Compounds, V. Balzari and V. Carassiti, Academic Press. Elements of Inorganic Photochemistry, G.J. Ferraudi, Wiley.
5. S.Arunachalam, "Inorganic Photochemistry - An Introduction to Photochemical andPhotophysical Aspects of Metal Complexes", Kala Publications, Tiruchirappalli, India, 2002.
6. D.M. Roundhill, “Photochemistry and photophysics of Metal complexes”, Springer;Edition, 1994.

MATERIALS CHEMISTRY

ELECTIVE-2C

Objective:

- *On completion of this course the students will have the knowledge of Principle involves in preparative technique, mainly, used to synthesize useful materials Importance of some useful properties of solid materials.*

Course Out comes

CO1: To Understand the role of materials and their classification
CO2: To know the preparative techniques of ceramic materials
CO3: The students gain the knowledge in superconductor materials
CO4: To study the functional organic materials of Fullerenes,ferroelectrics and organic superconductors
CO5: To know the importance of some useful properties of solid materials

UNIT-I MATERIAL DESIGN

Materials and their classification, Role of Chemistry in Material design. General methods of synthesis of inorganic materials—homogeneous nucleation and heterogeneous nucleation, growth of nuclei and factors of importance; synthesis of metallic, semiconductor and metal oxide nano particles.

UNIT-II PREPARATIVE TECHNIQUES

Ceramic methods; chemical strategies, chemical vapour deposition-MOCVD; preparation of nanomaterials, Langmuir- Blodgett Films. Fabrication of ordered nanostructures . Composition and purity of materials.

UNIT-III SUPERCONDUCTORS

Structural features of cuprate superconductors. 1-2-3 and 2-1-4 cuprates; structure. Normal state properties: anisotropy and temperature dependence of electrical resistance. Superconducting state: heat capacity, coherence length, relation between Tc and hole concentration in cuprates; mechanism of superconductivity in cuprates. Applications of high Tc-cuprates.

UNIT-IV FUNCTIONAL ORGANIC MATERIALS

Conducting organics - charge transfer materials and conducting polymers. Organic superconductors. Fullerenes. Molecular ferromagnets and ferroelectrics. Liquid crystals: mesomorphic behaviour, optical properties of liquid crystals, display devices.

UNIT-V NLO MATERIALS

Second and third order non-linear effects; molecular rectifiers and frequency doublers; unimolecular electronic devices. Photochromic materials; optical data storage, memory and switches.

Reference Books:

1. A.R. West, Solid State Chemistry and its Applications, (1984) John Wiley & Sons, Singapore.
2. T. V. Ramakrishnan and C.N.R. Rao, Superconductivity Today, (1992) Wiley. Eastern Ltd., New Delhi . N R. Rao and J. Gopalkrishnan, New Directions in Solid State Chemistry, (1997) Cambridge Univ. Press.
3. P. Ball, Designing the Molecular World: Chemistry at the Frontier, (1994) Princeton Univ. Press.

PRACTICAL-4

ORGANIC CHEMISTRY PRACTICAL - II

Course Objectives

- To understand the purifications techniques

Course Out come:

CO 1: Perform the ternary mixtures.
CO2: Preparation of organic compounds, their purifications and run TLC.
CO3: Determination of physical constant: Melting point, Boiling point.
CO4: Different separation techniques.
CO5: Extract, identify and characterize the compounds isolated from natural products

Any FOUR preparations from the following single stage preparations:

1. Preparation of p-benzoquinone from hydroquinone
2. p-Nitrobenzoic acid from p-nitrotoluene
3. Acetyl salicylic acid from salicylic acid
4. Benzhydrol from benzophenone
5. Preparation of 2,5-di-t-butylhydroquinone
6. 1,2,3,4 - Tetrahydrocarbazole from cyclohexanone
7. Preparation of dibenzylidene acetone
8. 2,3 - Dimethylindole from phenyl hydrazine and 2 - butanone

Any THREE preparations from the following involving two stages

1. sym-Tribromo benzene from aniline.
2. Benzanilide from benzophenone
3. m-Nitro benzoic acid from methyl benzoate
4. 2,4.- Dinitrobenzoic acid from p-nitrotoluene
5. m-Nitro benzoic acid from benzaldehyde
6. Phthalide from phthalic anhydride
7. 2-Phenyl indole from phenyl hydrazine
8. 2, 4-dinitrophenyl hydrazine from p-nitrochlorobenzene

Any TWO exercises in the extraction of natural products

Caffeine from tea leaves
Lactose from milk
Citric acid from lemon
Piperine from black pepper

Reference Books

1. Arthur I. Vogel, "A Textbook of Practical Organic Chemistry", ELBS.
2. N.S. Gnanapragasam and B. Ramamoorthy, "Organic Chemistry Lab Manual" (2006), S. Visvanathan Printers & Publishers.

PRACTICAL-5 INORGANIC CHEMISTRY PRACTICAL - II

Course Objectives

- To understand the anions and cations estimations techniques.

Course Out come:

CO 1: Identify various ions present in alloys.
CO2: Prepare and characterize various complexes and analyse the samples throughly.
CO3: Estimate the amount of ions by complexometric and gravimetric methods
CO4: To Know the Basic laws of Photochemistry.
CO5: Understand the concepts of various titrations of Complexometric methods.

Complexometric titrations

Estimation of Ca_{2+}, Mg_{2+}, Zn_{2+} and Ni_{2+} using EDTA
Determination of Hardness of water

Preparation of the followings:

Potassium tris (31xalate) aluminate (III) trihydrate
Tris (thiourea) copper (I) chloride
Potassium tris (oxalaato) chromate (III) trihydrate
Sodium bis(thiosulphato) cuprate (I)
Sodium hexanitrocobaltate (III)
Chloropentammine cobalt (III) chloride
Bis (acetylacetonato) copper (II)
Hexamminenickel (II) chloride
Bis (thiocyanato) pyridine manganese (II)

Colorimetric Analysis

Photoelectric method: Estimation of iron(III), nickel(III) and manganese(VII).

Reference Book

J.Mendham, R.C.Denney, J D Barnes, M. Thomas and B. Sivasankar, Vogel's text book of quantitative chemical analysis, Pearson Educaion Ltd., Indian subcontinent edition, 2009.

PRACTICAL-6 PHYSICAL CHEMISTRY PRACTICAL - II

Paper Code: TUCH27

Course Objectives:

- To understand the different techniques

Course Out come

CO 1: Determination of the equivalent conductancce of a wea acid at different concentrations and verify ostwls dilution law and calculate the dissociation constant f the acid.

CO2: Determianation of equivalent conductane of a strong electrolyte and verification of Debye- Huckel onsagar equation.

CO3: Verification of Ostwalss dilution law for a weak electrolyte.

CO4: Determination of Pka values of weak acids and weak bases.

CO5: Conductometric titrations of mixtures of two components. A. Acid - Base tutrations. B. precipitation titrations.

Conductometric Titrations:

1. Determination of the equivalent conductance of a weak acid at different concentrations and verify Ostwald's dilution law and calculate the dissociation constant of the acid.
2. Determination of equivalent conductance of a strong electrolyte at different concentrations and examine the validity of the Onsager's theory as limiting law at high dilutions.
3. Determination of equivalent conductance of a strong electrolyte and verification of Debye - Huckel - Onsager Equation
4. Verification of Ostwald's Dilution law for a weak electrolyte.
5. Determination of PK_a values of weak acids and weak bases.
6. Conductometric titrations of a mixture of acids (HCl, CH_3COOH) and NaOH.
7. Conductometric titrations of mixtures of two components.
   1. Acid-Base titrations.
   2. Precipitation titrations.
   3. C. Displacement titrations.
8. Mixture of halides

Reference Books

1. B.P.Levitt (Ed.), Findlay's Practical Physical Chemistry, 9_{th} edn., Longman, London,1985.
2. J.N.Gurtu and R.Kapoor, Advanced Experimental Chemistry, Vol.I, S.Chand & Co. Ltd., New Delhi, 1980.

SECOND YEAR: SEMESTER-III

CORE-7 ORGANIC CHEMISTRY-III
(Advanced Organic Chemistry)

Objectives:

- On successful completion of the course the students should have
- Learnt the basic principles of organic spectroscopy
- Learnt the structural analysis using spectral data
- Learnt the basic principles of photochemistry and electrocyclic reactions
- Learnt the pericyclic reactions.

Course Out come

CO 1: On successful completion of the course the students should have learnt the basic principles of organic spectroscopy, calculate the number of molecular weight using Woodward - Fieser rules and functional group identification.

CO2: On positive conclusion of the way the students should have well-read the basic principles of organic spectroscopy, calculate the number of proton and carbon present in the compound identification techniques also study in the unit.

CO3: On active completion of the progress the students should have Learn the mass spectrum and fragmentations techniques also study in the unit.

CO4: This unit explicates the plain theories of steroids hormones in organic synthesis. In calculation the students will advantage information on biosynthesis reaction mechanism.

CO5: This paper explicates the plain theories of alkaloids hormones in organic synthesis. In calculation the students will advantage information on biosynthesis reaction mechanism.

UNIT-I UV & IR

UV-Visible spectroscopy: Introduction- types of electronic transitions – chromophores and auxochromes – factors influencing positions and intensity of absorption bands, Woodward-Fieser rules for conjugated dienes, carbonyl compounds and enones, ultraviolet spectra of aromatic and heterocyclic compounds.

IR spectroscopy: Introduction- finger print region – Far IR region Applications of IR spectroscopy to identify alkane, alkene, alkyne, aromatic compounds, nitrile and aromatic residues, Identification of alcohols, ethers, phenols, amines and carbonyl compounds such as ketones, aldehydes, esters, amides, acids, conjugated carbonyls compounds and other functional groups- Effect of hydrogen bonding and effect of solvent on vibrational frequencies.

UNIT-II NMR

Introduction-Nuclear spin states- Nuclear Magnetic moments-Absorption of Energy-Resonance- Instrumentation: Continuous wave method, FT NMR-chemical shift and its measurements, factors affecting the chemical shift including anisotropic effect-relaxation processes-spin-spin coupling-coupling constant –multiplicity-spin systems-NOE effects-$_1$H NMR of simple aliphatic and aromatic compounds.

Principles of $_{13}$C NMR,- proton decoupled and off – resonance $_{13}$C NMR spectra – DEPT methods- factors affecting $_{13}$C chemical shift -$_{13}$C NMR spectra of simple organic molecules.

Problem solving (for molecules with a maximum number of C10).

UNIT-III MASS & PROBLEM SOLVING

Introduction- Principles- Instrumentation-Ionization techniques such as Chemical ionization, Electron ionization, ESI, FD, FAB, MALDI. Applications of mass spectra to elucidate molecular formula and structure. Mc. Lafferty rearrangement-Nitrogen rule-Interpretation of fragmentation pattern of aliphatic alcohols, aldehydes, esters, ethers, hydrocarbons, carboxylic acids, amines, halogen compounds and simple aromatic compounds. Appearance and significance of isotopic peaks.Structural elucidation of simple organic molecules with the application of spectral techniques- Problems involving combination of spectral data.

UNIT-IV SYNTHETIC METHODOLOGY

An introduction to synthons and synthetic equivalents, functional group interconversions, Planning and execution of multistep synthesis- overall yield calculation for multistep synthesis- synthesis of simple molecules. The importance of the order of events in organic synthesis, One group C-C disconnections – Alcohols and carbonyl compounds, regioselectivity, alkene synthesis, Olefination of carbonyl compounds, one group C-X and two group C-X disconnections, chemoselectivity, reversal of polaritiy, cyclization reactions, amine synthesis.

UNIT-V PHOTOCHEMISTRY AND PERICYCLIC REACTIONS

Principles of photochemical reactions; Photochemical excitation – fate of the excited molecules – Joblonski diagram – study of photochemical reactions of ketone – photoreduction – photocyclo addition – Paterno – Buchi reaction – di pi-methane and tri-pi methane rearrangement reaction. Pericyclic Analysis of electrocyclic, cyclo addition and sigmatropic reactions – correlation diagrams for butadiene – cyclobutene system, hexatriene systems. FMO and PMO approach, electrocyclic reactions, - conrotatory and dis rotatary motions, 4n, 4n+2 and allyl systems. Sigmatropic rearrangement, supra and antarafacial shifts of H Sigmatropic shifts involving carbon moieties, 3,3- and 5,5- sigmatropic rearrangement – Cope and Claisen rearrangement.

Reference Books

1. I.L. Finar, Organic Chemistry, Vol.II, Fifth edn. First Indian reprint, Pearson Education Asia Pvt. Ltd. 2000
2. P.S. Kalsi, Spectroscopy of Organic Compounds, Wiley Eastern Ltd. Madras, 1995.
3. Joseph Lambert, Scott Gronert, Herbert Shurvell, David Lightner, Robert Graham Cooks, Organic Structural Spectroscopy: Pearson New International Edition, 2_{nd} Edition, 2013.
4. William Kemp, NMR in Chemistry, Mac Millan, 1986.
5. R.O.C. Norman, Principles of Organic Synthesis, Second edn., Chapman and Hall, 1993.
6. R.K. Mackie, D. M.Smith and R.A. Aatkin, Guide Book to Organic Synthesis, 2_{nd} edn. Longman Scientific and Technical, London, 1990
7. S.Warren, Designing Organic Synthesis – A Programmed Introduction to Synthon Approach, Wiley, NY, 1978
8. R.O.C. Norman, Principles of Organic Synthesis, II Edn., Chapman and Hall, 1993.
9. Jaya singh and Jagadhamba singh, Photochemistry and Pericyclic reactions, New Age international Publishers, New Delhi, 2010.

CORE-8 **INORGANIC CHEMISTRY-III**

(Solid state, Bioinorganic and Nuclear Chemistry)

Objectives:
After completion of the course the students will have the knowledge of

- *Basic concepts describing structure of solids, Theories involves in diffraction by solids and properties of solids.*
- *Basis of nuclear moments and types of nuclear reactions*

Course Out come

CO 1: Know the Basic concepts of Solid State of Matter.
CO2: Know the theroies of Semiconductor,Insulatorand super conductors of Solids.
CO3: Understand the Concept of metal clusters in Coordination Compounds.
CO4: Acquire the fundamental knowledge in Nuclear Chemistry
CO5: Know the Working of Nuclear reaction in Nuclear Chemistry.

UNIT-I BASIC CONCEPTS IN SOLID STATE

Lattice, unit cell, crystal systems and Bravais lattices-Miller indices and labelling of planes –symmetry properties –crystallographic point groups and space groups –fundamentals of X-ray diffraction- Laue equation and Brag's law-powder and single crystal X-ray diffraction-Scherrer formula-systematic absences, reciprocal lattice-structure factor and intensity- electron density maps- electron and neutron diffraction.

UNIT-II INORGANIC SOLIDS

Structures of rock salt –cesium chloride-wurtzite –zinc blende –rutile –fluroite –antifluorite-diamond and graphite –spinel –normal and inverse spinels and perovskite –lattice energy of ionic crystals –Madelung constant-Born-Haber cycle and its applications. Defects- types of defects-non – stochiometry – point defects in solids – Schottky and Frenkel defects- colour centers – linear defects –dislocations – effects due to dislocations- Metallic state – free electron and band theories- insulator, semiconductor, -intrinsic and extrinsic semi conductors- Types of magnetic behaviours of solids.

UNIT-III BIO-INORGANIC CHEMISTRY

Transport proteins-Oxygen carriers-metalloenzymes, carboxy peptidase, carbonic anhydrase, redox process, iron-sulphur proteins, chlorophyll- salient features of the photo synthetic process- vitamin B12-the role of sodium, potassium, calcium, zinc and copper-sodium-potassium pumps- fixation of nitrogen, nitrogen cycle.

UNIT-IV NUCLEAR CHEMISTRY-1

Nuclear properties: Nuclear spin and moments, origin of nuclear forces, salient features of the liquid drop and the shell models of the nucleus. Models of Radioactive Decay: Orbital electron capture: nuclear isomerism, internal conversion, detection and determination of activity by cloud chamber, nuclear emulsion, bubble chamber, G.M., Scintillation and Cherenkov counters. Nuclear Reactions: Types, reactions, cross section, Q-value, threshold energy, compound nucleus theory: high energy nuclear reactions, nuclear fission and

fusion reactions as energy sources; direct reactions; photonuclear and thermo nuclear reactions.

UNIT-V NUCLEAR CHEMISTRY-2

Stellar energy: synthesis of elements, hydrogen burning, carbon burning, Nuclear Reactors: fast breeder reactors, particle accelerators, linear accelerators, cyclotron and synchrotron.

Radio Analytical Methods: Isotope dilution analysis, Radiometric Titrations, Radio 36mmune assay, Neutron activation analysis.

Reference Books

1. West, A. R. Solid State Chemistry and its Applications, John Wiley & Sons: New York, 1989
2. L.V.Azaroff – Introduction to solids, John Wiley.
3. W.E.Addision – structural principles of Inorganic Chemistry, Longman, 1961.
4. N.B.Hannay – Solid state chemistry, Prentice Hall, New Delhi, 1976.
5. R.A.Alberty and Silby – Solid state chemistry.
6. S.Glasstone – Source book on atomic energy, Von Nostrand Co., 1969.
7. G.Friedlander, J.W.Kennedy, - Nuclear and Radiochemistry, John Wiley and sons, 1981.
8. H.J.Arnikar – Essentials of Nuclear chemistry, Wiley Easter Co., 4_{th} edition, 1995.
9. S. J. Lippard and J. M. Berg, Principles of Bioinorganic Chemistry, Panima Publishing Company, New Delhi, 1997.
10. W. Kaim and B. Schewederski, Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life , John Wiley & Sons, New York, USA.
11. C. N. R. Rao and J.Gopalakrishnan, New Directions in Solid State Chemistry.

CORE-9 **PHYSICAL CHEMISTRY-III**

(Electrochemistry and Spectroscopy)

Objectives:

After this course the student should be able

- *To understand the behavior of electrolytes in solution.*
- *To know the structure of the electrode surface.To differentiate electrode kinetics from other types kinetic studies.To make the students knowledgeable in nuclear chemistry.*
- *To learn the applications of spectroscopy for the study and structural 37lucidate ion of molecules.*
- *To apply the principles of mass, UV-Visible, IR, NMR, ESR, Photo electron spectroscopy.*
- *To know the application of spectroscopy to study the structure of molecules.*

Course Out come

CO 1: The behavior of electrolytes in solution
CO2: The structure of the electrode surface
CO3: Tifferenctiate electrode kinetics from others types kinetic studies
CO4: the application of spectroscopy for the study and structural elucidate ion of molecules.
CO5: principles of mass, UV, IR, NMR, ESR, photo electronspectroscopy.

UNIT-I ELECTROCHEMISTRY-I

Kohlrausch law and its applications-Debye-Huckel-Onsagar equation-Derivation-validity of DHO equation-deviation of DHO equation-conductance of high field and high frequency-Electro kinetic phenomena-Electro capillary phenomenon-Lipmann's equation-Zeta potential and its applications.
Introduction to electrical double layer-Evidences for electrical double layer.
Structure of electrified interface-Helmholtz-Perrin, Guoy-Chapmann and Stern models of electrical double layer.

UNIT-II ELECTROCHEMISTRY-II

Overpotential-Elementary electron electrode process. Butler-Volmer equation-Exchange current density and symmetry factor-Experimental determinations-Electrode rectification. Nernst equation as a special case of Butler-Volmer equation—Reaction resistance-Polarisable & non-polarisable electrodes-Low and high field approximations-Tafel equations. Corrosion and its prevention. Fuel cells-Classification-Chemistry of fuel cells-detailed description-ion-selective electrodes.

UNIT-III PHASE RULE AND SPECTROSCOPY-I

Phase equilibria-Gibb's phase rule-Condensed systems-Application to three component systems-Graphical representation-Systems of three liquids-System consisting of two salts and water-Perihydric and cryohydric systems.
Classification of molecules-Rigid rotor model-Effect of isotopic substitution on the transition frequencies-Non-rigid rotor-Applications-Vibrational energies of diatomic molecules-zero point energy-force constant and bond strengths-anharmonicity-vibration-rotaional spectroscopy-P,Q,R branches-Vibration of poly atomic molecules-overtones-hot bands-far-IR region-Fermi-resonance.

UNIT-IV SPECTROSCOPY-II

Classical and quantum theories of Raman effect-Stokes' and anti-Stokes' lines-Raman selection rules.
Rotational Raman spectra- linear molecules, symmetric top and spherical top molecules; Vibrational Raman spectra-symmetry and Raman active vibrations, rule of mutual exclusion; Rotation-Vibration Raman spectra of diatomic molecules. Resonance Raman spectroscopy-Coherent anti-Stokes Raman Spectrosocpy (CARS)-Applications.

UNIT-V PHOTOCHEMISTRY

Franck-Condon principle-Jablonskii diagram-primary and secondary processes-Flourescence and phosphorescence-Quantum yield-Chemical actionometry-Photosensitization, chemiluminescence-kinetics of unimolecular photophysical processes-Kinetics of photochemical processes-H_2 and Cl_2 reaction-Excimers and Exciplexes. Mechanism of fluorescence quenching- Stern-Volmer equation and its applications.Photo-Voltaic cells-Photo-assisted electrolysis of water-Aspects of solar energy conversion.

Reference Books

1. J.O.M. Bokris and A. K. N. Reddy, Electrochemistry, Vol. 1 and 2, Plenum, New York.
2. S. Glasstone, Introduction to Electrochemistry, Affiliated East West Press, New Delhi.
3. D.R.Crow, Principles and Applications to Electrochemistry, Chapman and Hall (1991).
4. H.Reiger, Electrochemistry, Prentice-Hall International Inc, New York (2012).
5. R. Chang – Basic principles of spectroscopy, McGraw Hill, New Delhi.
6. C.N. Banwell and E.N. McCash – Fundamentals of Molecular spectroscopy, 5th Edition, Tata McGraw Hill, New Delhi, 2006.
7. G.M. Barrow, Introduction to Molecular Spectroscopy, Mc Graw Hill, New York, 2007.
8. N.J.Turro, Modern Molecular Photochemistry, Benjamin, Cumming, Menlo Park, California.
9. K.K.Rohatgi, Mukherjee, Fundamentals of Photochemistry, New Age International Pvt. Ltd, Chennai, 2009.
10. R.P.Wayne, Photochemistry, Butterworths, London.

ELECTIVE-3A GREEN AND SUSTAINABLE CHEMISTRY

Objectives:
After this course the student should be able

- *To understand the advantages and importance of green chemistry.*
- *To look for green chemistry strategies for designing the chemical synthesis.*
- *To know the solvent free synthesis using MWI.*
- *To make the students knowledgeable in solar energy conversion.*

Course Out come

CO 1: To understand the advantages and importyance of green chemistry.
CO2: To look for green chemistry strategies for designing the chemical synthesis.
CO3: To make the students knowledgable in solar energy conversion.
CO4: To understand the basics of water chemistry.
CO5: To understand the importance of polymers in industries.

UNIT-I GREEN CHEMISTRY

Introduction: Prospects and future of Green Chemistry, Twelve guiding principles of green chemistry. Concept of atom economy. Green starting materials, Green reagents, Green solvents and reaction conditions, Green synthesis- Real world cases (Traditional Vs. Green processes) Synthesis of Ibuprofen, Adipic acid. Biomimetic, multifunctional reagents; Combinatorial green chemistry; Non-covalent derivatization.

UNIT-II GREEN TECHNOLOGIES

Green Solvents: Enhancement of selectivity, efficiency, and industrial applicability-Ionic liquids-Supercritical fluids-Solvent free neat reactions in liquid phase-Flourous phase reactions
Green Catalysis: Heterogeneous catalysis: Use of zeolites, silica, alumina, clay, polymers, cyclodextrins, and biocatalysts.

UNIT-III MICROWAVE AND ULTRASOUND MEDIATED ORGANIC SYNTHESIS

Microwave assisted reactions, Microwave activation – advantage of microwave exposure – specific effects of microwave – Neat reactions – solid supported reactions _ Functional group transformations – condensation reactions – oxidation – reduction reactions – multi-component reactions.
Ultrasound assisted reactions, ultrasound for waste water treatment, cleaning and organic synthesis– oxidation– reduction reactions.

UNIT-IV IONIC LIQUIDS AND PTC

Introduction – synthesis of ionic liquids – physical properties – applications in alkylation – hydroformylations– epoxidations – synthesis of ethers – Friedel-craft reactions – Diels-Alder reactions – Knoevengal condensations – Wittig reactions – Phase transfer catalyst - Synthesis – applications.

UNIT-V NEW ENERGY SOURCES FOR NEW CENTURY

Renewable energy sources-Introduction to solar energy- Biomass conversion-Sea wave energy-tidal energy-geo-thermal energy-wind energy-nuclear fusion energy. Splitting of water-hydrogen from sunlight-hydrogen economy.
Fuel cells-batteries-photovoltaic cells. Nuclear energy-Nuclear fission and fusion-Production of electricity by nuclear reactor-radioactivity and hazards of radioactivity-living with nuclear power-Management of radioactive waste.

Reference Books

1. Environmental Pollution, A.K. De
2. Mike Lancaster , Green Chemistry and Introductory text, II Edition
3. P.T.Anastas and J.C Warner,Green Chemistry theory and Practice, Oxford University press, Oxford (1988).
4. V.K. Ahluwalia, Methods and Reagents of Green Chemistry: An Introduction by Green Chemistry, Ane Books India, 2006.
5. Green Chemistry – Environment friendly alternatives- edited by Rashmi Sanghi & M. M. Srivastava, Narora Publishing House, (2003).

ELECTIVE-3B SURFACE ANALYTICAL TECHNIQUES & SENSORS

Objectives:
After this course the student should be able

- *To understand the principles of ECSA, SERS and other techniques.*
- *To know the principles and application of electroanalytical techniques.*
- *To apply the student knowledge in the importance of sensor*
- *To make the student knowledgeable in the application of biosensors.*

Course Out come

CO 1: To understand the principles of ECSA, SERS and other techniques
CO2: To know the principles and application of electroanalytical techniques
CO3: To apply the student knowledge in the importance of sensor
CO4: To make the students knowledgable in the application of biosensors
CO5: The students to gain the knowledge in Electrochemical sensors and Biosensors

UNIT-I SURFACE ANALYTICAL TECHNIQUES-1

Electron Spectroscopy for Chemical Analysis (ESCA): Principles, Instrumentation, and Analytical Applications. Auger electron spectroscopy: Principles, Instrumentation, Applications. Secondary ion mass spectrometry (SIMS):Principles, Instrumentation, Applications.

Surface enhanced Raman Spectroscopy (SERS): Principles, Instrumentation, Nanoparticulate SERS substrates, Surface enhanced resonance Raman scattering (SERRS), SERRS of Ag and Au metal colloids, Thin solid films, Langmuir-Blodgett Monolayers.

UNIT-II SURFACE ANALYTICAL TECHNIQUES-2

Mapping and imaging, Applications. Electron Energy Loss Spectroscopy (EELS): Principles, Instrumentation, Applications. Electron Microprobe analysis: Principles, Instrumentation, Analysis of semiconductors and crystalline materials, Applications. Low Energy Ion Scattering Spectroscopy: Principle, Instrumentation, Surface structural analysis.

UNIT-III CHEMICAL SENSORS

Importance of Sensors, Biomolecular recognition elements, Artificial molecular-recognition materials, Molecular imprinted polymers, Electrode modification. Fluorescence, chemi and bio-luminescence sensors, Fluorescent tag molecules, Applications.

UNIT-IV ELECTROCHEMICAL SENSORS

Conductometric sensors, Coulometric sensors, Voltammetric sensors, Applications, Neurotransmitters, Amperometric sensors, Chronoamperometric analysis, Multichannel sensors, Microelectrode sensors, Electrochemical Impedance Sensors, Quartz crystal nanobalance sensors.

UNIT-V BIOSENSORS

Molecular recognition, Applications. Surface Plasmon resonance based sensors, Fiber optic sensors, Two dimensional microarray based sensors, Applications for Food Safety – Mycotoxins, adultrants, Biomedical diagnosis – Cancer markers.

Reference Books

1. Brian R. Eggins, Chemical Sensors and Biosensors, Analytical Techniques in the Sciences (ANTS), 2nd Edition, Wiley, 2002.
2. Gabor Harsanyi, Sensors in Biomedical Applications – Fundamentals, Technology and Applications, CRC Press, 2000.
3. Raluca-Ioana Stefan, Electrochemical Sensors in Bioanalysis, CRC Press, 2001.
4. D J O'Connor, Brett A Sexton, Roger S C Smart (Eds), Surface Analysis Methods in Materials Science, 2nd Edition, Springer, 2010.
5. John C Vikerman, Ian Gilmore (Eds.), Surface Analysis: The Principal Techniques, 2nd Edition, Wiley, 2009.
6. John F Watts, John Wolstenholme, An Introduction to Surface Analysis by XPS and AES, 2nd Edition, Wiley VCH, 2011.

ELCETIVE3C COMPUTATIONAL METHODS IN CHEMISTRY AND HEMOMETRICS

Objectives:

After this course the student should be able

- *To understand the basic knowledge of use of computer in chemistry.*
- *To know the software use in drawing the chemical structures.*
- *To apply the student knowledge in chemometrics.*
- *To make the student knowledgeable in the application of numerical methods of analysis.*

Course Out come:

CO 1: To understand the basic knowledge of use of computer in chemistry
CO2: To know the software use in drawing the chemical structures
CO3: To apply the students knowledgeable in the application of mumerical methods of analysis
CO4: To apply the student knowledge in chemometrics
CO5: The students to gain the knowledge in computational methods in chemistry and chemometrics

UNIT-I COMPUTER BASICS

Windows and Linux; MSOFFICE; Statistical Data Processing and Curve Fitting by EXCEL, GRAPHER, SURFER and MATHEMATICA; Chemical Structure Drawing by ISIS Draw, CHEMWIND, ACD Labs and
CHEMDRAW; Molecular Modeling by ACD Labs, PCWIN and CHEM 3D; Chemical Databases; Animations and Virtual Chemical Experiments

UNIT-II FORTRAN 77

Types of Constants and Variables in Fortran, Dimension, Data, Type, COMMON and EQUIVALENCE statements, Arithmetic and Logical IF, IF-THEN ELSE Constructs, DO statement, Various types of I/O statements, Library functions, Statement functions, Function subprograms and subroutine subprograms with suitable examples.

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, Least square curve fitting.

UNIT-IV COMPUTER APPLICATION

Role of computer in research, data organization, software selection and its applications, solving problems by using scientific software & tools, sample programmes for analysis of data.
Computer Searches of Literature: ASAP Alerts, CA Alerts, SciFinder, ChemPort, ScienceDirect , STN International-Journal home pages.

UNIT-V CHEMOMETRICS

Introduction to Chemometrics, principles of experimental design, factorial and fractional factorial design, specific applications. Response surface methodology and Optimization, Response surface designs, Sequential optimization, specific, numerical problems. Modelling and Knowledge processing: multiple linear regressions, test parameter estimation, PCR, PLS, PCA etc. Cluster analysis and descriminant analysis, 42odeling of multiway regression.

Reference Books

1. V. Rajaraman, Fortran 77, Prentice Hall (India), New Delhi.
2. S.D. Conte and C. deBoor, Elementary Numerical Analysis, McGraw-Hill (Intl. Edition) (1987).
3. K. V. Raman, Computers in Chemistry, Tata McGraw Hill (1993).
4. E. Morgan, Chemometrics: Experimental Design, John Wiley & Sons, 2008.
2. Otto Mattias, Chemometrics: Statistics and Computer Application in Analytical Chemistry, Wiley, 2007
3. J.N. Miller and J. C. Miller, Statistics and Chemometrics for Analytical Chemistry, Pearson Prentice Hall, 6_{th} Edition, 2010.
4. Brereton, R.G, Chemometrics: Data Analysis for the Laboratory and Chemical Part, Wiley, 2003.

PRACTICAL-7 ORGANIC CHEMISTRY PRACTICAL – III

Course Objectives:

- To understand the separations techniques

Course Out come

CO 1: To understand the Column, Paper, Thin Layer Chromatography

CO2: To know about the High Performance Thin Layer Chromatography

CO3: To familiarize the two dimensional Paper Chromatography, Reverse phase paper chomatography.

CO4: To learn about the Gas-liquid Chromatography

CO5: To know about the High Performance Liquid chromatography

Chromatographic Separations

Column chromatography - separation of anthracene and picric acid from anthracene picrate.
Thin layer chromatography separation of green leaf pigments.
Paper chromatography-Identification of amino acid.

Any FOUR Estimations

Estimation of aniline
Estimation of phenol
Estimation of glucose
Estimation of amino group
Estimation of amide group
Saponification of fat or oil
Iodine value of an oil
Estimation of sulphur in an organic compound
Estimation of methyl ketone

Special Interpretation Of Organic Compounds-UV, IR, PMR and MASS Spectra of the following 15 compounds

1, 3, 5- Trimethyl benzene
Pinacolane
n-Propylamine
p-Methoxy benzyl alcohol
Benzyl bromide
Phenylacetone
2-Methoxyethyl acetate
Acetone
Isoopropyl alcohol
Acetaldehyde diacetate
2-N,N-Dimethylamino ethanol
Pyridine
4-Picoline
1,3-dibromo-1,1-dichloropropene
Cinnamaldehyde

Reference Books

1. Arthur I.Vogel, A text book of Practical Organic Chemistry, ELBS
2. Raj K. Bansal, Laboratory Manual of Organic Chemistry, Wiley Eastern limited.
3. N.N. Greenwood and A. Earnshaw, Chemistry of the Elements, Vol.II, Pergamon Press (1997).
4. R. M. Silverstein, F. X. Webster, D. J. Kiemle. Spectrometric Identification of Organic Compounds, Seventh Edition.

PRACTICAL-8 INORGANIC CHEMISTRY PRACTICAL - III

Analysis of Alloys

Estimation of tin and lead in solder.
Estimation of copper and zinc in brass/Bronze.
Estimation of chromium and nickel in stainless steel.

Analysis of Ores

Dolomite, Galena, Pyrolusite, Copper pyrites

Quantitative Analysis

Quantitative analysis of mixtures of iron –magnesium; iron – nickel; copper – nickel and copper – zinc.

List of Spectra to be given for interpretation.

$_{31}P$ NMR Spectra of methylphosphate
^{31}P NMR Spectra of HPF_2
^{19}F NMR Spectra of CIF_3
$_1H$ NMR Spectra of Tris (ethylthioacetanato) cobalt (III)

Explain high resolution $_1H$ NMR spectra of (N-propylisonitrosoacetylacetoneuninato) (acetylacetonato) Nickel (II)
ESR Spectra of the aqueous $ON(SO_3)_{2-}$ ion.
ESR Spectra of the H atoms in CaF_2.
ESR Spectra of the $[Mn\ (H_2O)_6]^{2+}$.
ESR Spectra of the bis (salicylaldiminato) copper (II)
IR Spectra of the sulphato ligand.
IR Spectra of the dimethylglyoxime ligand and its Nickel (II) complex.
IR Spectra of carbonyls
Mossbauer spectra of $FeSO_4.7H_2O$
Mossbauer spectra of $FeCl_3$.
Mossbauer spectra of $[Fe(CN)_6]_{3-}$
Mossbauer spectra of $[Fe(CN)_6]_{4-}$

Reference Book

J.Mendham, R.C.Denney, J D Barnes, M. Thomas and B. Sivasankar, Vogel's text book of quantitative chemical analysis, Pearson Educaion Ltd., Indian subcontinent edition, 2009.

PRACTICAL - 9

PHYSICAL CHEMISTRY PRACTICAL - III

1. Potentiometric titrations of a mixture of acids.
2. Precipitation titrations- $AgNO_3$ vs. KCl.
3. Determination of pH and calculation of pKa.
4. Determination of the dissociation constant of weak acid using quinhydrone/calomel electrode.
5. Determination of strength of KI using potentiometric titration between FAS and KI.
6. Determination of strength of FAS using potentiometric titration between $KmnO_4$ and FAS.
7. Experiment on precipitation titration of mixture of halides by EMF measurements.

Spectral Interpretation:

Experiments given only to familiarize the interpretation of spectra provided. Interpretation of simple UV-Visible spectra of simple molecules for the calculation of molecular data and identification of functional groups (5 typical spectra will be provided).

IR and NMR spectral calculations of force constant – identification and interpretation of a spectra (5 each in IR and NMR will be provided).

Reference Books

1. Findlay`s practical Physical Chemistry, `Revised and edited by B.P. Levitt, 9_{th} edn., Longman, London, 1985.
2. J.N,Gurtur and R.Kapoor,"Advanced Experimental Chemistry," Vol.I, S.Chand & Co., Ltd., New Delhi.
3. Practical Physical Chemistry by B. Viswanathan and P.S. Raghavan, Viva publishers.

SEMESTER-IV

CORE-10 SCIENTIFIC RESEARCH METHODOLOGY

Objectives:

- *To study about the importance of research, literature survey, error analysis, statistical treatment.*
- *To know the various indexes and abstracts in science and technology as a source of in format ion in chemistry.*
- *To study about the conventions of writing thesis.*

UNIT-I MEANING OF RESEARCH

Nature and importance of research-aims, objective, principles and problems-selection of research problems, purpose of research, scientific method, role of theory, characteristics of research. Types of research: fundamental or pure research, applied research, action research, historical research, experimental research.

UNIT-II CHEMICAL LITERATURE

Sources of chemical information: primary, secondary and tertiary sources. Indexes and abstracts in science and technology: applied science and technology index, chemical abstracts, chemical titles, current chemical reactions, current contents, physics abstracts, science citation index. Beilstein compilations of data, synthetic methods and techniques, treatises, reviews.

UNIT-III CHEMICAL ABSTRACTS

Current awareness searching: CA weekly issues, CA issue indexes. Retrospect ive searching: CA volume indexes-general subject index, chemical substance index, formula index, index of ring systems, author index, patent index. CA Collective indexes: Collective index (CI), decennial index (DI).

Access points for searching CA indexes: index guide, general subject terms, chemical substance names, molecular formulas, ring systems, author names, patent numbers. Locating the reference: finding the abstract, finding the original document, chemical abstract service source index.

UNIT-IV SCIENTIFIC WRITING

Scientific writings: research reports, theses, journal articles, and books.

Requirement of technical communications: eliminating wordiness and jargon tautology, redundancy, imprecise words, super fluous phrases.

Steps to publishing a scientific article in a journal: types of publications communications, articles, reviews; when to publish, where to publish, specific format required for submission, organization of the material. Documenting: abstracts-indicative or descriptive abstract , informative abstract, footnotes, end notes, referencing styles, bibliography-journal abbreviations (CASSI),abbreviations used in scientific writing.

UNIT-V COMPUTER SEARCHES OF LITERATURE

ASAP Alerts, CA Alerts, SciFinder, ChemPort, ScienceDirect , STN International Journal home pages.

Reference Books

1. R. L. Dominoswki, Research Methods, Prentice Hall, 1981.
2. J. W.Best, Research in Education, 4th ed. Prentice Hall of India, New Delhi, 1981.
3. H. F. Ebel, C. Bliefert and W. E. Russey, The Art of Scientific Writing, VCH, Weinheim, 1988.
4. B. E. Cain, The Basis of Technical Communicating, ACS., Washington, D.C., 1988.
5. H. M. Kanare, Writing the Laboratory Notebook; American Chemical Society: Washington, DC, 1985.
6. J. S. Dodd, Ed., The ACS Style Guide: A Manual for Authors and Editors; American Chemical Society: Washington, DC,1985.
7. Gibaldi, J. Achtert, W. S. Handbook for writers of Research Papers; 2nd ed.; Wiley Eastern, 1987.
8. Joseph, A. Methodology for Research; Theological Publications: Bangalore, 1986.

CORE-11 BIO-ORGANIC AND HETEROCYCLIC CHEMISTRY

UNIT-I PROTEINS AND NUCLEIC ACIDS

Proteins: Peptides and their synthesis – Merrifield synthesis, Determination of N-terminal/C-terminal residues, Determination of tertiary structure of Protein, Bio-Synthesis of Proteins. Nucleic Acids: Types of Nucleic Acids-DNA & RNA polynucleotide chain. Components-biological functions. Structure and role of (genetic Code) DNA and RNA (Nucleotides only).

UNIT-II STEROIDS

Occurrence, nomenclature, basic skeleton, Diel's hydrocarbon and stereochemistry, Isolation, structure determination and synthesis of Cholesterol, Bile acids, Conversion of cholesterol into sex hormones such as androsterone, testosterone, estrone and progesterone. Biosynthesis of Cholesterol.

UNIT-III THREE AND FOUR MEMBERED HETEROCYCLES

Systematic nomenclature (Hantzsch-Widman system) for monocyclic, fused and bridged heterocycles. Three-membered and four-membered heterocycles-synthesis and reactions of aziridines, oxiranes, thiranes, azetidines, oxetanes, thietanes –Corey-Chaykovsky reaction, Darzens glycidic ester condensation, Hoch-Campbell aziridine synthesis, Jacobsen.Katsuki epoxidation.

UNIT-IV FIVE AND SIX MEMBERED HETEROCYCLICS

Synthesis and reactions of furan, pyrrole, thiophene and pyridines: Furans-Fiest Benary furan synthesis, Knorr and Paal-Knorr pyrrole synthesis, Pyrroles and pyrrolidines-Barton. Zard reaction. Hofmann-Loffler-Freytag reaction. Thiophenes-Hinsberg synthesis of thiophene derivatives. Oxazoles and isoxazoles- Robinson-Gabriel synthesis, Cook – Heilbron 5-amino-thiazole synthesis. Hurd.Mori 1,2,3-thiadiazole synthesis. Pyridines- Hantzsch (Dihydro)-pyridine synthesis. Skraup/Doebner von Miller reaction. Chichibabin (Tschitschibabin) pyridine synthesis.

UNIT-V CONDENSED HETEROCYCLES

Synthesis and reactions of benzopyrroles, benzofurans and benzothiophenes, Indoles. Indoles-Fischer indole synthesis, Madelung indole synthesis, Nenitzescu indole synthesis. Quinolines and isoquinolines- Bischler-Napieralski reaction. Friedlander synthesis. Meth-Cohn quinoline synthesis. Pfitzinger quinoline synthesis. Pyrralo-pyrroles, Furanopyrroles thienopyrroles, Coumarins, chromones, quinolizinium ions.

Reference Books

1. Heterocyclic Chemistry, J.A. Joule, K. Mills, Blackwell ,Science, Cambridge, 4_{th} edition, 2000.
2. Organic Chemistry , Jonathan Clayden, Nick Greeves, Stuart Warren, and Peter Wothers, Oxford University Press, 2000.
3. Heterocyclic Chemistry Vol. 1-3, R.R. Gupta, M. Kumar and V. Gupta, Springer Verlag, New York, 1999.
4. The Chemistry of Heterocycles. T Eicher and S. Hauptmann. (Series: Organic Chemistry Monographs.) Thieme, Stuttgart,. 1996. 504 pp.
5. Heterocyclic Chemistry, T.L. Gilchrist, Longman Scietific Techinal, New York, 3_{rd} edition, 1997.
6. Comprehensive Heterocyclic Chemistry, A.R. Katritzky and C.W. Rees, E. F. V. Scriven. Pergamon Press, Elsevier, New York 1996, Vol 2,
7. Natural Products: Their Chemistry and Biological Significance., J. Mann, R. S. Davidson, J. B. Hobbs, D. V. Banthrope, J. B. Harborne, Longman Scientific and Technical (Wiley), New York, 1994.
8. Advanced Organic Chemistry: Structure and Mechanisms (Part A &B). Frances A Carey and Richard J Sundberg, Springer, 2007.
9. Heterocyclic chemistry, R. K. Bansal, Wiley India Pvt Ltd,, 4_{th} edition, 2008..
10. Name reactions in heterocyclic chemistry-By Jie Jack Li, E. J. Corey Contributor Jie Jack Li, Published by John Wiley and Sons, 2004.

ELECTIVE-4A **APPLICATION OF ANALYTICAL TECHNIQUES TO INORGANIC COMPOUNDS**

Objectives:

- *On the completion the course the students will have the knowledge of various analytical techniques.*
- *Insight into the concepts and interpretation of spectra of IR, Raman, NMR, EPR, Mossbauer, and NQR to characterise the Inorganic compounds*

UNIT-I INFRARED AND RAMAN SPECTROSCOPY

Structural studies (involving IR and Raman spectroscopy) of coordination compounds containing the following molecules/ions and ligands - NH_3, H_2O, OH^-, SO_4^{2-}, CN^-, SCN–, NO, O_2, PR_3 and halides

UNIT-II NMR SPECTROSCOPY

Different spin systems – chemical shifts and coupling constants (spin-spin coupling)involving different nuclei ($_1H$, $_{19}F$, $_{31}P$, $_{13}C$) interpretation and applications to inorganic compounds – Effect of quadrupolar nuclei ($_2H$, $_{10}B$, $_{11}B$) on the $_1H$ NMR spectra, Satellite spectra. Systems with chemical exchange - evaluation of thermodynamic parameters in simple systems – study of fluxional behavior of molecules – an elementary treatment of second order spectra – examples – NMR of paramagnetic molecules – isotropic shifts contact and pseudo-contact interactions – Lanthanide shift reagents.

UNIT-III EPR SPECTROSCOPY

Theory of EPR spectroscopy - Spin densities and McConnell relationship – Factors affecting the magnitude of g and A tensors in metal species - Zero-field splitting and Kramers degeneracy – Spectra of VO(II), Mn(II), Fe(II), Co(II), Ni(II) and Cu(II) complexes – Applications of EPR to a few biological molecules containing Cu(II) and Fe(III) ions.

Magnetic properties:
Types of magnetism – Dia –para – ferro and antiferro magnetism. Magnetic properties of free ions – first order Zeeman effect – Second order Zeeman effect – states KT – states<<KT. Determination of Magnetic moments and their applications to the elucidation of structures of inorganic compounds – temperature independent paramagnetism. Magnetic properties of lanthanides and actinides. Spin crossover in coordination compounds.

UNIT-IV MOSSBAUER SPECTROSCOPY

Principle-Isomer shifts – Magnetic interactions – Mossbauer emission spectroscopy – applications to iron and tin compounds.

UNIT-V NQR SPECTROSCOPY

Characteristics of quadrupolar nucleus – effects of field gradient and magnetic field upon quadrupolar energy levels – NQR transitions – applications of NQR spectroscopy.

Reference Books

1. R.S. Drago, Physical Methods in Inorganic Chemistry, 3rd Ed., Wiley Eastern Company .
2. R.S.Drago, Physical Methods in Chemistry, W.B. Saunders Company, Philadelphia, London.
3. F.A. Cotton and G.Wilkinson, Advanced Inorganic Chemistry, 3rd ed., Wiley-Eastern Company, New Delhi 1990.
4. P.J. Wheatley, The Determination of Molecular Structure, .
5. Lewis and Wilkins, Modern Coordination Chemistry,.
6. E.A.V.Ebsworth, Structural Methods in Inorganic Chemistry, 3rd ed., ELBS, Great Britain, 1987.

ELECTIVE-4B INSTRUMENTAL METHODS OF ANALYSIS

Objectives:

- *On the completion the course the students will have the knowledge of various instrumental techniques.*
- *The students should have learnt data analysis and electro analytical techniques.*

UNIT-I DATA ANALYSIS

Definition of Terms – Mean, Median, Precision and accuracy; Errors in chemical analysis- systematic errors and random errors. Treatment of data – Basic statistical concepts and frequency distribution, Average and measure of dispersion; Significance of Gaussian distribution curves; Null hypothesis; confidence interval of mean, Criteria for rejection of data; Regression and correlation; quality control and control chart.

UNIT-II OPTICAL METHODS OF ANALYSIS

Absorption spectrometry – Beer Lamberts law; Spectrophotometry: UV visible spectroscopy- photometric titrations; Fluorimetry, turbidimetry and nephelometry.

Flame Photometry–Theory, instrumentation and a few important applications; Atomic absorption spectroscopy (AAS) – Theory, instrumentation and applications; Atomic fluorescence.Infra-red spectroscopy – Theory and instrumentation – source, monochromators, detectors; dispersive and non dispersive instruments; sample handling techniques; qualitative analysis and quantitative applications.

Raman spectroscopy – Theory, instrumentation – source of radiation and detectors; few qualitative and quantitative applications; Resonance Raman spectroscopy.

UNIT-III NMR, ESR AND MOSSBAUER SPECTROSCOPY

Nuclear Magnetic Resonance Spectroscopy –Theory, relaxation and saturation processes, Environmental effects; instrumentation – type of magnets, source, detector and sample handling; few application of proton NMR; qualitative and quantitative analysis.

Electron Spin Resonance –Theory, instrumentation and a few applications in qualitative and quantitative analyses.

Massbauer spectroscopy: principle, instrumentation – applications; molecular structure, isomerism, electronic structure.

UNIT-IV POLAROGRAPHY, AMPEROMETRY AND CHROMATGRAPHY

Polarography – Theory, apparatus, DME, diffusion kinetic catalytic currents, current voltage curves for reversible and irreversible system, qualitative and quantitative application to inorganic systems.

Amperometric titrations – Theory, apparatus, types of titration curves, successive titrations and two indicator electrodes-applications.

TLC, Colum, gas, ion exchange, Gel permeation, Gas liquid chromatography-principle, retention time values, instrumentation, carrier gas, column, detectors- thermal conductivity, flame ionization and electron capture; few applications of GLC.

UNIT-V RADIOCHEMICAL METHODS

Hot atom chemistry – the Szilard – chalmers process, chemistry of recoil atoms, chemical effects no radiative decay, solvated electron. Uses of radiations in the study of matter, neutron activation analysis, dilution analysis, dosimetry, synthesis of organic and inorganic compounds by irradiation, radiometric analysis, radiography.

Reference Books

1. Willard, Merit, Dean and Settle, Instrumental Methods of Analysis, CBS Publishers and Distributors, IV Edn. 1986
2. Schoog, Holler, Nieman, Principles of Instrumental Analysis, Thomson Asia Pte Ltd., Singapore, 2004.
3. D.A. Skoog and D.M. West Fundamentals of Analytical Chemistry, Holt Rinehart and Winston Publications, IV Edn, 2004.
4. W. Kemp, NMR in Chemistry, MacMillan Ltd,1986.

ELECTIVE-4C ENVIRONMENTAL CHEMISTRY

Objectives:
After this course the student should be able

- *To understand the basic knowledge of natural cycles in the environment.*
- *To know the various pollutants affecting environment.*
- *To apply the student knowledge in preventing pollution.*

UNIT-I INTRODUCTION TO ENVIRONMENTAL CHEMISTRY

Concept and scope of environmental chemistry, Environmental terminology and nomenclatures, Environmental segments, The natural cycles of environment (Hydrological, Oxygen, Nitrogen, Phosphorous and Sulphur cycles).

UNIT-II ATMOSPHERE

Regions of the atmosphere, Reactions in atmospheric chemistry, Earth's radiation balance, Particles, ion and radicals in the atmosphere, stratospheric chemistry: The chemistry of ozone layer, The role of chemicals in ozone destruction, The green-house effect and Global warming, El-Nino phenomenon.

UNIT-III LITHOSPHERE

The terrestrial environment, Soil formations, Soil properties (physical/chemical), inorganic and organic components in soil, acid-base and ion-exchange reactions in soil, micro and macro nutrients, nitrogen pathways and NPK in soil, waste and pollutants in soil, waste classification and disposal.

UNIT-IV AIR POLLUTION

Air pollutants (sources, classification, sampling and monitoring): Particulates, Aerosols, SO_X, NO_X, CO_X and hydrocarbon emission, Photochemical smog, Autoexhausts, Acid-rains, Air-quality standards. Method of control of air pollution: Method of control of air pollution, electrostatic precipitation wet & dries scrubber, filters, gravity and cyclonic separation, Adsorption, absorption and condensation of gaseous effluent

UNIT-V WATER POLLUTION

Water pollutants (sources, sampling and monitoring), Water-quality parameters and standards: physical and chemical parameters (colour, odour, taste and turbidity), Dissolved oxygen, BOD, COD, Total organic carbon, Total nitrogen, Total sulfur, Total phosphorus and Chlorine, Chemical speciation. Method of control of water pollution: Water and waste water treatment, aerobic and anaerobic, aeration of water, principle of coagulation, flocculation, softening, disinfection, demineralization and fluoridation.

Reference Books

1. G.W. Vanloon, S.J. Duffer, Environmental Chemistry – A Global Perspective, (2000) Oxford University Press.
2. F.W. Fifield and W.P.J. Hairens, Environmental Analytical Chemistry, 2nd Edition (2000), Black Well Science Ltd.)
3. Colin Baird, Environmental Chemistry, (1995) W.H. Freeman and Company, New York.
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.
7. S.K. Banerji, Environmental Chemistry, 1st Edition (1993), Prentice-Hall of India, New Delhi.

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CORE-12 PROJECT

Field of Project – Organic / Inorganic / Physical Chemistry
No. of hours/week 20
No. of Credit 10

Supervisor & research topic:

The guide and area of research should be allotted to each student before the end of third semester. Each guide shall have a maximum of five students.

Plan of Work:

The student should prepare the plan of project work with due consultation of guide and get the approval of the Head of the Department. In case the student wants to avail the facility from other University/laboratory, they will undertake the work with the permission of the guide and acknowledge the facilities utilized by them.

The duration of the dissertation research shall be a minimum of three months in the fourth semester.

Dissertation Work outside the Department:

In case the student stays away for work from the Department for more than one month, specific approval of the Head of the Department should be obtained.

No. of copies of dissertation:

The students should prepare four copies of dissertation and submit the same for the evaluation by Examiners. After evaluation, one copy is to be retained in the Department library and one copy is to be submitted to the University (COE) and one copy each can be held by the guide and student.

Format to be followed:

The format/certificates for dissertation to be submitted by the students are given below:

Format for the preparation of project work:

(a) Title page

(b) Certificate from the guide

(c) Declaration of Student

(d) Acknowledgement

(e) Table of contents

CONTENTS

Note :

1. Blue colour indicates the syllabus change.
2. Red colour indicates the Job oppournity from various chemical industries.