

THIRUVALLUVAR UNIVERSITY

SERKKADU, VELLORE – 632 115

DEPARTMENT OF CHEMISTRY



MASTER OF SCIENCE IN CHEMISTRY

[Under Choice Based Credit System (CBCS)]

w.e.f the academic year 2020-21

SYLLABUS AND REGULATIONS

FOR UNIVERSITY DEPARTMENT

ABOUT THE DEPARTMENT

The department of chemistry was established in 2002 as post-graduate and 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, 1 administrative staff, 32 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

Chemistry provides immense scope for study, research and gainful employment in various sectors. The Department of Chemistry of Thiruvalluvar University is determined to educate and graduate rural students. The department is 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 2020-21)

The course of study and scheme of examinations

1. TITLE: M.Sc., Chemistry

2. YEAR OF IMPLEMENTATION: July 2020 onwards

3. COURSE DETAILS:

Total No. of Semesters	- 04 (Two semesters per year)
No. of theory papers per semester	- 05/06
Total No. of theory papers	- 21
No. of practical courses per semester	- 02 (upto III semester)
Total No. of Practicals	- 06
Project	- IV semester

Total Marks for M.Sc. Degree

Theory	- 2100 marks
Practicals	- 600 marks
Project	- 100 marks
Total	-2800 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 board of studies revised the syllabus of M.Sc., Chemistry in 2018 and the new revised syllabus covers broad area of fundamental aspects in modern chemistry.

The syllabi are all set to meet the standard of CSIR-UGC-NET, GATE 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 than 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

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

The question papers will be set by the internal and the scrutiny of the question paper will be done by external. Evaluation of answer scripts will be done by internal.

- **Internal Assessment**

Test	: 10 marks (best 2 out of 3)
Assignment	: 10 Marks
Seminar	: 05 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 75 marks each for university examination and 25 marks for internal evaluation.

Distribution of marks for practical examinations

University Examination Experiment : 75 Marks

Procedure	: 5 marks
Experiment	: 30 marks
Interpretation	: 10 marks
Result	: 10marks)
Practical viva-voce	: 10 marks
Record	: 10 Marks
Total	: 75 marks

Practical Internal Assessment

Number of Experiments	: 10 marks
Performance	: 10 Marks
Test	: 5 Marks
Total	: 25 marks

Passing Minimum in practical examinations

IA	: 12 Marks (50 %)
UE	: 38 Marks (50 %)
Total	: 50 Marks

All the practical examinations will be conducted for 6 hours only i.e. 10 AM – 4PM by both the internal examiners.

- For the project report

Report	: 75 marks
Viva-voce	: 25 marks
Total	: 100 Marks

Distribution of marks for project report (Total of 100 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 - 75 marks

(Dissertation Format – 10 marks; Scope of the research problem – 20 marks; Methodology – 20 marks; Analysis – 10 marks, Results and findings-15 marks)

Viva-Voce examination – 25 marks

(Presentation – 10 marks; subject knowledge – 10 marks; Interaction – 5 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 Examination-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 (2018-19 to 2020-21), 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.

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The course of study and scheme of examinations

Subject	Paper Code	General Title	Ins. Hrs./ Week	Credit	Exam hrs	Max. Marks		
						IA	UE	Total
1st Year: I Semester								
Core-1	TUCH11	Organic Chemistry – I	5	4	3	25	75	100
Core-2	TUCH12	Inorganic Chemistry – I	5	4	3	25	75	100
Core-3	TUCH13	Physical Chemistry – I	5	4	3	25	75	100
Elective -1	TUCH14A	A. Medicinal and Heterocyclic Chemistry OR	5	3	3	25	75	100
	TUCH14B	B. Chemistry of Macromolecules OR						
	TUCH14C	C. Organic Analytical Techniques						
	TUCH15VAC	Value added course	2	2	3	25	75	100
Practical-1	TUCH16	Inorganic Chemistry Practical - I	4	4	6	25	75	100
Practical-2	TUCH17	Physical Chemistry Practical - I	4	4	6	25	75	100
			30	25		175	525	700
1st Year: II Semester								
Core-4	TUCH21	Organic Chemistry – II	5	4	3	25	75	100
Core-5	TUCH22	Inorganic Chemistry - II	5	3	3	25	75	100
Core-6	TUCH23	Physical Chemistry – II	5	4	3	25	75	100
Compulsory	TUHR20	Human Rights	2	2	3	25	75	100
Elective -2	TUCH24A	A. Supramolecular and Nano Chemistry OR	3	3	3	25	75	100
	TUCH24B	B. Inorganic Photochemistry OR						
	TUCH24C	C. Materials Chemistry						
Open Elective for Non-Major students	TUCH25OEA	Industrial chemistry	2	2	3	25	75	100
	TUCH25OEB	Medicinal and Agricultural chemistry						
	TUCH25OEC	Nano chemistry						
Practical-3	TUCH25	Organic Chemistry Practical – I	4	4	6	25	75	100
Practical-4	TUCH27	Physical Chemistry Practical – II	4	4	6	25	75	100
			30	26		200	600	800

Subject	Paper Code	General Title	Ins. Hrs. /Week	Credit	Exam hrs	Max. Marks		
						IA	UE	Total
2nd Year: III Semester								
Core-7	TUCH31	Organic Chemistry – III	5	4	3	25	75	100
Core-8	TUCH32	Inorganic Chemistry – III	5	4	3	25	75	100
Core-9	TUCH33	Physical Chemistry – III	5	3	3	25	75	100
Elective -3	TUCH34A	C. Green and Industrial Chemistry OR	5	3	3	25	75	100
	TUCH34B	B. Surface Analytical Techniques and Chemical, Electrochemical and Biosensors OR						
	TUCH34C	C. Computational Methods in Chemistry and Chemometrics						
Practical-5	TUCH35	Organic Chemistry Practical – II	4	4	6	25	75	100
Practical-6	TUCH36	Inorganic Chemistry Practical -II	4	4	6	25	75	100
Open Elective for Non-Major students Open Elective - 2		Chemistry in day to day life	2	2	3	25	75	100
		Radiation Chemistry and Spectroscopy						
		Chemistry of Biomolecules						
		MOOC Course	-	2	3	25	75	100
		USSR	-	2		25	75	100
			30	28		225	675	900
2nd Year: IV Semester								
Core-10	TUCH41	Organic Chemistry-IV	4	4	3	25	75	100
Core-11	TUCH42	Scientific Research Methodology	4	3	3	25	75	100
Elective-4	TUCH43A	A. Applications of Spectral Techniques to Inorganic Compounds OR	4	3	3	25	75	100
	TUCH43B	B. Instrumental Methods of Analysis OR						
	TUCH43C	C. Environmental Chemistry						
Core-12	TUCH44	Project	18	5	-	25	75	100
			30	15		100	300	400
Total			120	94				2800

*IA = Internal Assessment

*UE = University Examination

Core (11 Theory Papers + 6 Practicals)

: 65 Credits - 1700 marks

Elective (4 Theory Papers) + 2 Open Elective + MOOC Course + USSR

: 20 Credits - 800 marks

Compulsory Paper (Human Rights) + Value added course

: 04 Credits - 200 marks

Project
Total

: 05 Credits - 100 marks
: 94 Credits - 2800 Marks

FIRST YEAR **SEMESTER-I**

CORE-1

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

Paper Code: TUCH11

Total hours : 75

Objectives:

- *On successful completion of the course, the students should have a versatile knowledge of aromaticity and to understand the principles and reaction mechanism involving various reactive intermediates.*
- *The course also aims to explain basic concepts in stereochemistry and conformational analysis of organic molecules.*

UNIT-I AROMATICITY

Generalization of Aromaticity: Hückel's $4n + 2$ Rule, Craig's rule, Aromatic, Anti-aromatic and Non-aromatic Systems. Aromaticity of benzenoid and non-benzenoid compounds, Annulenes; Fulvenes and Related Systems. Ions-Cations, Anions- Cross-conjugated 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 and spiranes. 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. Stereochemistry of cis and trans decalines, hydrindanes and cyclohexene.

UNIT-IV REACTIVE INTERMEDIATES

Carbocations, carbanions, free radicals, radical cations, radical anions, carbenes and nitrenes, arynes – generation, stability: factors affecting stability (carbocation and carbanion), 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, 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, Stereochemistry 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, 5thEdn., Vol.2, Stereochemistry and Chemistry of Natural Products, Pearson, 2014.
T.L. Gilchrist and C.W. Rees, Carbenes, Nitrenes and Arynes, Thomas Nelson and Sons Ltd., London.

CORE-2

INORGANIC CHEMISTRY-I

(Main Group and Coordination Chemistry)

Paper Code: TUCH12

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 structure, stability and reactivity of coordination complexes.*

UNIT-I MAIN GROUP CHEMISTRY-1

VSEPR- $d\pi-p\pi$ bonding, Bent's rule; Theories of acid and base. The HSAB concept. Theoretical basis of hardness and softness. Structure and bonding of boranes-diborane and higher boranes, borazines, S-N compounds, phosphazenes and cyclic phosphazene, silicates and silicones; Interhalogen and Noble gas compounds- Hybridisation, Geometry and properties.

UNIT-II THEORIES OF COORDINATION CHEMISTRY

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-III STRUCTURE OF COORDINATION COMPLEXES

Structures 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.

UNIT-IV SUBSTITUTION REACTIONS

Substitution reactions in square planar complexes – Trans effect- Theories of trans effect – the factors affected by square planar complexes - Reaction mechanism and kinetics of nucleophilic substitution in octahedral complexes – the factors affected by octahedral complexes- acid bases hydrolysis – conjugate base mechanism - reaction rates influenced by acid and bases.

UNIT-V STABILITY OF COMPLEXES AND ELECTRON TRANSFER REACTIONS

Labile and inert complexes- stepwise and overall stability of complexes – factors affecting stability of complexes-methods of determination of stability constant (Job's and potentiometric methods)

Mechanisms of electron transfer reactions - outer sphere mechanisms - excited state outer sphere electron transfer reactions - inner sphere mechanisms – atom transfer reaction-Marcus-Hush theory- mixed valent complexes-

Reference Books

1. Inorganic Chemistry - Principles of structure and reactivity, Fourth Edition, J. E. Huheey, E. A. Keiter and R. L. Keiter - Addison 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. Pearson
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 Chemical Kinetics)****Paper Code: TUCH13***Objectives:*

- *To know the limitations of classical thermodynamics in the evaluation of macroscopic properties.*
- *To understand the principles of activity and fugacity.*
- *To know the theories of kinetic activity.*
- *To study the techniques of fast reactions.*
- *To learn about the various surface phenomena.*

UNIT-I THERMODYNAMICS AND NON-IDEAL SYSTEMS

Concepts of Partial Molar Properties-Partial Molar Free Energy and Partial Molar Volume. Chemical potential-Variation of chemical potential with temperature and pressure, Van't Hoff isotherm.

Fugacity-Determination of fugacity of gases by graphical method-Variation of fugacity with temperature and pressure -Lewis Randal rule-Duhem-Margules equation. Determination of activity and activity coefficient of non-electrolyte (EMF method)-Excess functions.

UNIT-II IRREVERSIBLE THERMODYNAMICS

Nernst heat theorem-Third law of thermodynamics-Applications of third law-Entropy change-Calculation of absolute entropies-Apparent exceptions to third law- Non-equilibrium thermodynamics-Basic concepts-Forces and fluxes-Entropy of irreversible processes-Entropy production-Clausius inequality-Phenomenological equations-Onsager reciprocity relations-Coupled reactions.

UNIT-III CHEMICAL KINETICS-I

Potential energy surfaces and Contour diagrams-Microscopic reversibility - Steady-state approximation- Theory of Absolute Reaction Rates- Probability factor-Comparison of transition state theory with collision theory-Eyring equation-Significance of entropy and enthalpy of activation-Linear free energy relationships (LFER) -Hammett and Taft equations-Kinetic isotopic effect.

UNIT-IV CHEMICAL KINETICS-II

Application of ARRT to reaction in solutions - Influence of ionic strength (Bjerrum-Bronsted equation) and dielectric constant on rates in solution- Acid-Base catalysis-Mechanism-Bronsted catalysis law. Kinetics of consecutive reactions.

Enzyme Catalysis-Michaelis-Menten equation-Effect of pH and temperature on enzyme catalyzed reactions-Inhibition of enzyme catalyzed reactions
Fast reactions-Laser Flash photolysis, flow technique and relaxation methods.

UNIT-V SURFACE CHEMISTRY AND CATALYSIS

Chemisorption and Physisorption; Langmuir's adsorption isotherm; - Mechanisms of reactions on surfaces (Rideal-Eley and Langmuir-Hinshelwood mechanisms); BET isotherm-BET equation-Estimation of surface area.

Surface active agents-Classification of surface active agents, Micelles and Reverse Micelles-Critical Micellar Concentration (CMC), Factor affecting the CMC of surfactants.

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 thermodynamics, Benjamin publishers, California, 1972.
4. R. Hasee, Thermodynamics of Irreversible Process, Addition Wesley, Reading.
5. Thomas Engel and Philip Reid, Physical Chemistry, Third Edition, Pearson, 2014.
6. P.W. Atkins, Physical Chemistry, 7thedn, Oxford University press, 2002.
7. K.J. Laidler, Chemical Kinetics, Pearson, 5th edition, 2011.
8. J. Rajaram and J.C. Kuriacose, Kinetics and Mechanisms of chemical transformations: Application to Femtochemistry, McMillan, 2011.
9. Agarwal, Basic chemical kinetics, Tata McGraw-Hill, 1990.
10. R.G. Frost and Pearson, Kinetics and mechanism, Wiley, New York.
11. A.W. Adamson, Physical chemistry of surfaces, 6th Ed., Wiley, 1997.
12. G.A. Somorjai, Introduction to surface chemistry and catalysis, John Wiley, 1994.
13. Maron and Prutton, Principles of physical chemistry, McMillan.
14. W.J. Moore, Physical Chemistry, Orient Longman, London (1972).

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.*

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.

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

Pro drug concept: prodrugs of ampicillin, elanapril, propranolol.

UNIT-III DRUG ACTION

Pharmacological activity – Antibiotics: Penicillin; Antimalarials: Trimethoprim; NSAIDS: Paracetamol, Ibuprofen, Diclophenac sodium, Antidepressants: Fluoxetine, Anti-histamines, Anti-tuberculosis agents: Isoniazide, Anti-cancer agents: Vinblastine, Taxol

Unit-IV HETEROCYCLICS

Synthesis and reactions of furan, pyrrole, thiophene and pyridines: Furans-Fischer-Benary furan synthesis, Pyrroles and pyrrolidines-Barton. Zard reaction. Hofmann-Löffler-Freytag reaction. Thiophenes-Hinsberg synthesis of thiophene derivatives. Pyridines- Hantzsch (Dihydro)-pyridine synthesis. Skraup/Doebner von Miller reaction.

UNIT-V CONDENSED HETEROCYCLES

Synthesis and reactions of Indole, Quinolines and Isoquinolines: 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.

Reference Books

1. Burger's Medicinal Chemistry & Drug discovery, Vol 1-3, 5th Ed, 1995.
2. Chemistry of drug design and drug action-. R. B. Silverman (2004) Acad. press.
3. Graham Patrick, An Introduction to Medicinal Chemistry- 2ndEdn. 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

CHEMISTRY OF MACROMOLECULES

Paper Code: TUCH14B

Objective:

- *To gain the knowledge in the preparation, properties, characterization and Uses of polymers and biomacromolecules*

UNIT – I INTRODUCTION AND SYNTHESSES OF MACROMOLECULES

Introduction, Colloids, Macromolecules, Synthetic Polymers, Biological Polymers, Macromolecular Science.

Techniques of polymerization: emulsion, bulk, solution and suspension. Mechanism of polymerization : free radical, cationic, anionic and co-ordination polymerization (Ziegler - Natta Catalyst), Living Polymers, Coordination Polymerization, Stepwise Polymerization.

UNIT – II STRUCTURE AND PROPERTIES

Structure - property relationship – Mechanical properties, Thermal properties – Glass transition temperature – Factors affecting Glass transition temperature – crystallinity and melting point – related to structure.

B) Polymer characterization and analysis

Crystalline nature – X-Ray diffraction – Differential Scanning Calorimetry (DSC) – Thermo Gravimetric Analysis – molecular weight determination – Osmometry (membrane), Viscosity, Ultra centrifuge and Gel Permeation Chromatography.

UNIT III LIQUID CRYSTALS POLYMERS

Mesogens, Polymeric Liquid Crystals, Low-Molecular Weight Liquid Crystals, Main-Chain Liquid-Crystalline Polymers, Side-Chain Liquid-Crystalline Polymers, Segmented-Chain Liquid-Crystalline Polymers.

UNIT – IV INDUSTRIAL NATURAL POLYMERS

Important industrial polymers – preparation and application of polyethylene, poly vinyl chloride, poly urethanes, polytetrafluoro ethylene (TEFLON), Nafion and ion – exchange resins.

Importance of natural polymers – application and structures of starch, cellulose and chitosin derivatives.

UNIT-V 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).

Text Books:

1. F. W. Bill Meyer. Text book of polymer science, III Edition, John Wiley and sons, New York.
2. P. J. Flory. Principles of Polymer Chemistry, Cornell Press (recent edition).
3. V. R. Gowariker, B. Viswanathan, J. Sridhar, Polymer Science – Wiley Eastern, 1986.
4. G. S. Misra – Introduction to Polymer Chemistry, Wiley Eastern Ltd.,
5. P. Bahadur, N. V. Sastry, Principles of Polymer Science, Narosa Publishing House.
6. G. Odian, Principles of Polymerization, McGraw Hill Book Company, New York, 1973.

ELECTIVE – 1C ORGANIC ANALYTICAL TECHNIQUES

Paper Code: TUCH14C

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.*

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, vacuum distillations. Recrystallization, Sublimation.

UNIT-II EXTRACTION TECHNIQUES

Solvent extraction: Principle and techniques. Distribution ratio and distribution coefficient. Factors affecting extraction efficiency: 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),. 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. Paper electrophoresis.

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
G. D. Christian and J.E.O Reilly, Instrumental Analysis, Allyn and Bacon Inc, II Edn., 1986.

PRACTICAL - 1

INORGANIC CHEMISTRY PRACTICAL – I

Paper Code: TUCH16

Semimicro qualitative analysis of inorganic mixture containing two common and two rare earth cations.

The following are the rare earth cations to be identified.

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

Complexometric titrations

Estimation of Ca^{2+} , Mg^{2+} , Zn^{2+} and Ni^{2+} using EDTA

Preparation of the followings:

Potassium tris (oxalate) aluminate (III) trihydrate

Tris (thiourea) copper (I) chloride

Potassium tris (oxalato) 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 Books

PRACTICAL- 2 PHYSICAL CHEMISTRY PRACTICAL – I

Paper Code: TUCH17

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 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 I₂.
12. Distribution of acetic acid between water and chloroform.
13. Decomposition of diacetone alcohol-dilatometry method.
14. Complex formation by spectrophotometry-Job's method.

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, "AdvancedExperiemental 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 and named reactions 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.*

UNIT-I OXIDATION AND REDUCTION REACTIONS

Oxidation: Carbon Oxidation Number -Calculation. Study of the following oxidation reactions: chromium trioxide, Osmium tetroxide, DDQ, Chloranil-Alkenes to epoxides and dihydroxy compounds; Oxidation of alcohols using PCC, PDC, Jones, Dess-Martin oxidation; Sharplessepoxidation, Oppenauer oxidation, Oxidation using $\text{Pb}(\text{OAc})_4$, 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-II SUBSTITUTION REACTIONS

Aliphatic Substitution Reactions: Mechanism of aliphatic substitution reactions - $\text{S}_{\text{N}}1$, $\text{S}_{\text{N}}2$, $\text{S}_{\text{N}}i$, mechanism- non-classical carbocations-Neighboring group participation. Substitution at carbonyl, vinylic and bridgehead systems - substitution by ambident nucleophiles- HVZ reaction, Stark-Enamine reaction.

Aromatic Substitutions: Electrophilic substitution-the arenium ion mechanism. Orientation and reactivity (ortho, meta and para directing groups). Typical reactions including Vilsmeier - Haack, Schiemann 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-III 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-IV MOLECULAR REARRANGEMENTS

A detailed study with suitable examples of the mechanism of the following rearrangements: Wagner - Meerwein, Demjanov, Dienone - phenol, Favorski, Baeyer - Villiger, Sommet Hauser, Pummerer and Von Richter rearrangements.

UNIT-V NAMED REACTIONS AND REAGENTS IN ORGANIC SYNTHESIS

Reagents: Lithium dialkylcuprates, lithium diisopropylamide(LDA), Dicyclohexylcarbodiimide(DCC), Trimethylsilyl iodide. Named Reactions: Mannich reaction, Biginelli Reaction, Perkin reaction, McMurry coupling, Robinson annulation, Bischler-Napieralski reaction, Polonowski reaction, Bucherer reaction, Willegerodt and Willegerodt-Kindler reaction.

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, Mechanism and Structures in Organic Chemistry, Holt, New York (1959).

Organometallic compounds in catalytic reactions – classification- oxidative addition- reductive elimination- insertion- migration- nucleophilic substitution- reactions of coordinated ligands - isomerisation of alkenes- hydrogenation(Wilkinson's catalyst) –hydroformylation (oxo process)- oxidation of olefins(Wacker process) - 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, Berlin, 1985.
4. Inorganic Chemistry - Principles 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
7. B. Cornils and W.A> Herrmann, Applied homogeneous catalysis, Wiley VCH, Weinheim, 2002.
8. R.B. Jordan, Reaction mechanism of Inorganic and organometallic system, Oxford University press, oxford, 1991.
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.

CORE-6

PHYSICAL CHEMISTRY-II

(GROUP THEORY, SPECTROSCOPY and QUANTUM CHEMISTRY)

Paper Code: TUCH23

Objectives:

- Learn about the various principles and applications involved in group theory.
- To know the knowledge about the construction of character tables.
- To understand the principles and selection rules for IR and Raman spectroscopy and symmetry of hybrid orbital's.
- To become familiar with the required mathematics for operators and their applications in quantum mechanical problems.

- *To become familiar with the required mathematics for solving quantum mechanical problems.*
- *To learn the applications of spectroscopy for the study and structural elucidation of molecules.*
- *To apply the principles of UV-Visible, IR, and Raman spectroscopy.*

UNIT-I GROUP THEORY

Definition of groups, subgroups, Abelian and non-Abelian groups-Multiplication tables-Representation of cyclic groups-Similarity transformation- Symmetry elements and symmetry operations, matrix representation-point groups, Schönflies notations, Matrix representations - reducible and irreducible representations, characters of representations. Direct product representation. Great Orthogonality Theorem (without proof).

UNIT-II GROUP THEORY AND ITS APPLICATIONS

Construction of character tables using GOT for C_{2v} , C_{3v} and D_{2h} . 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-III PHASE RULE AND SPECTROSCOPY-I

Phase Rule : Derivation of Gibb's phase rule. Application to three components system-Graphical representation-Systems of three liquids (Chloroform/acetic acid/water; water/silvernitrate/ammonium nitrate). Classification of molecules (linear, symmetric top and asymmetric top molecules)-Rigid rotor model-Effect of isotopic substitution-Non-rigid rotor-Applications-Vibrational energy expression-zero point energy-force constant and bond strengths-anharmonicity; vibration-rotational spectroscopy-P,Q,R branches-overtone-hot bands-Fermi-resonance; far-IR region.

UNIT-IV SPECTROSCOPY-II

Classical and quantum theories of Raman effect-Stokes' and anti-Stokes' lines-Raman selection rules.

Rotational Raman spectra-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 Spectroscopy (CARS)-Applications.

UNIT-V QUANTUM CHEMISTRY-I

Wave-particle dualism, Uncertainty principle. Black body radiation, Planck's radiation law-Photoelectric effect-Compton effect.

Spherical polar co-ordinates-Postulates of quantum mechanics. Diagrams of radial and angular wave functions. Radial and angular distribution function and their significance.

Operators: Algebra operator, Commutation operator, Linear and Hermitian operator, Hamiltonian operator- Angular momentum operator -eigen functions and eigen values- Physical significance of wave function.

Schrödinger equation-Applications of Schrödinger equation to simple systems-Particle in a box-one and three-dimensional box problem-Orthogonalisation and normalisation-QM tunneling.

Reference Books

1. F.A. Cotton, Chemical application of Group theory, 3rd Edition John-Wiley & Sons, Singapore, 2003.
2. K.V. Raman, Group theory and its applications to chemistry, Tata McGraw-Hill, 1994.
3. V. Ramakrishnan and M.S. Gopinathan, Group theory in chemistry, Vishal publications, 1998.
4. Bhattacharya, Group theory and its applications, Himalaya Publishing House, 1992.
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, McGraw Hill, New York, 2007.
8. Gordon M. Barrow-Physical Chemistry, McGraw Hill Publishing Company Ltd., 2007.
9. R.K. Prasad, Quantum chemistry, Wiley Eastern, 1993.
10. W. Levine, Quantum chemistry, Prentice-Hall, 2000.
11. D.A. McQuarrie, Quantum chemistry, University science books, MilValley, California, 1998.
12. P.W. Atkins, Molecular Quantum mechanics, Clarendon Press New York, 2009.
13. R. Anantharaman, Fundamentals of Quantum chemistry, McMillan India.
14. Thomas Engel and Philip Reid, Quantum Chemistry and Spectroscopy, Pearson, 6th edition, 2012.

15. A. K. Chandra, Introductory quantum chemistry, 4th ed., Tata McGraw Hill 1994.
16. H.K. Moudgil, Text Book of Physical Chemistry, PHI Learning, New Delhi, 2010.

ELECTIVE-2A

SUPRAMOLECULAR AND NANO CHEMISTRY

Paper Code: TUCH24A

Objectives:

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

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 framework 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 ZnO₂, TiO₂, silver, gold, rhodium, palladium, platinum, and; carbon materials- fullerene- porous nano carbon(PNC)-synthesis

Techniques of synthesis: electroplating and electro-phoretic deposition, conversion through chemical reactions 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-desorption 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

Paper Code: TUCH24B

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.*

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 candidates, (2,2-bipyridine and 1,10-phenanthroline complexes), illustration of reducing and oxidising character of $[\text{Ru}(\text{bipy})_3]^{2+}$ complex, comparison with $[\text{Fe}(\text{bipy})_3]^{2+}$; 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 and Photophysical Aspects of Metal Complexes", Kala Publications, Tiruchirappalli, India, 2002.
6. D.M. Roundhill, "Photochemistry and photophysics of Metal complexes", Springer;Edition, 1994.

ELECTIVE-2C

MATERIALS CHEMISTRY

Paper Code: TUCH24C

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

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 T_c and hole concentration in cuprates; mechanism of superconductivity in cuprates. Applications of high T_c -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. C.N R. Rao and J. Gopalkrishnan, New Directions in Solid State Chemistry, (1997) Cambridge Univ. Press.
3. T. V. Ramakrishnan and C.N.R. Rao, Superconductivity Today, (1992) Wiley Eastern Ltd., New Delhi.
4. P. Ball, Designing the Molecular World: Chemistry at the Frontier, (1994) Princeton Univ. Press.

Open elective 10E1

MEDICINAL AND AGRICULTURAL CHEMISTRY

(for Non-major Students)

TUCH250EA

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.*

UNIT-I Drug Discovery and Design

History of drug discovery, Introduction to drugs and receptors, Drug-Receptor interactions, Neurotransmitters-Neurotransmission. Drug design strategies-rational drug design: Inhibitors of ACE; structure based drug design: Anti HIV agents.

UNIT-II Drug Action

Basics about DNA and RNA. DNA replication, Genetic code translation and transcription.

Pharmacological activity – Antibiotics: Penicillin; Antimalerials: Sulfa drugs, Trimethoprim; NSAIDS: Paracetamol, Ibuprofen, Diclophenac sodium, Antidepressants: Fluoxetine, Anti-cancer agents: Vinblastine, Taxol.

Unit III Pharmaceutical Analysis

Principles, instrumentation and applications to the following: Absorption spectroscopy (UV-Visible & IR). Principles and applications of chromatographic methods – TLC, HPLC and GC.

UNIT-IV Fertilizers

Details about indigenous fertilizer production, raw materials, details of the various nutrients with their importance. Source of nitrogen and hydrogen, steam reforming of hydrocarbons. Partial oxidation of Fuel oils, with gas purification which includes high and low temperature shift conversion, CO₂ removal processes and methanation.

Unit-V Pesticides

Chemistry of Pesticides: Brief introduction to classes of pesticides (Chemical class, targets), structures, chemical names, physical properties, chemical properties.

Entry and distribution of different classes of pesticides in plants and animals. Pesticide metabolism – microsomal oxidation, cytochrome P450 interaction, extra microsomal metabolism, enzymatic conjugation. Metabolism of different classes of pesticides involving different enzyme systems.

Reference Books

1. Burger's Medicinal Chemistry & Drug discovery, Vol 1-3, 5th Ed, 1995.
2. Chemistry of drug design and drug action-. R. B. Silverman (2004) Acad. press.
3. Graham Patrick, An Introduction to Medicinal Chemistry- 2ndEdn. Qxford, 2010

Open elective 1OE2

INDUSTRIAL CHEMISTRY

Objective

To enable the students to understand the principle of chemical technology and to utilize the raw materials in chemical industry.

Unit I Principles of Chemical Technology

Introduction: Basic principles – importance – classification – designing and modeling of chemical plants – unit process and unit operations.

Basic requirements of industrial reactors – choice and selectivity of reactor – basic principles of homogeneous and heterogeneous processes and reactors with examples.

Unit II Raw Materials and Energy for Chemical Industry

Raw materials – Characteristics of raw materials and their resources – methods of raw material concentrations – integral utilization of raw materials.

Energy for chemical industry – Fuels – classification of fuels – coal – fuel gases and liquid fuels – petroleum – cracking – Octane number – cetane number – composition and uses of coal gas, water gas, producer gas, oil gas and gobar gas.

Unit III Cement, Ceramics, Glass and Fertilizers

Cement: Manufacture – Wet Process and Dry process. Types, Analysis of major constituents, setting of cement, reinforced concrete. Cement industries in India.

Ceramics: Important clays and feldspar, glazing and verification.

Glass: Types, Composition, manufacture of Optical glass, colored glasses, lead glass and neutron absorbing glass.

Fertilizers: Fertilizer industries in India, Manufacture of ammonia, ammonium salts, urea, superphosphate, triple superphosphate and nitrate salts.

Unit IV Small Scale Chemical Industries

Electrothermal and electrochemical industries: electroplating – surface coating industries – oils, fats and waxes – soaps and detergents – cosmetics. Match industries and fire works: manufacture of some industrially important chemicals like potassium chlorate, and red phosphorus – metal powders.

Unit V Sugar and Agro Chemical

Sugar: Cane sugar manufacture, recovery of sugar from molasses, sugar estimation, sugar industries in India.

Agrochemical industries: Important categories of insecticides, fungicides, herbicides. Mode of action and synthesis of common pesticides like Gammexane, DDT, alathrin, Parathion, Malathion, Baygon, DDVP, Warfarin.

Reference Books

1. I.Mukhlyonov(ed.), Chemical Technology, Vol.1, Mir publication, Moscow, III edn., 1979.

2. A.K.De., Environmental Chemistry, Wiley Eastern Ltd., 11 edn., Meerut 1989. Chs 5-7
3. B.K Sharma – Industrial chemistry – Goel publishing house.
4. R.Norris Shreve and J.A.Brink, Jr. Chemical Process Industries. IV edn., McGraw Hill, Tokyo, 1977.
5. B.N.Chakrabarty, Industrial Chemistry, Oxford & IBH Publishing Co., New Delhi, 1981.
6. P.P.Singh, T.M.Joseph, R.G.Dhavale, College Industrial Chemistry, Himalaya Publishing House, Bombay, 4th edn., 1983.

Open Elective 1OE3

NANOSCIENCE AND GREEN CHEMISTRY

TUCH25OEC

Objective

To understand the basic concept of nano science and green chemistry.

Unit I

Characterization and synthesis of nano particles

Introduction – importance and characterization of nanomaterials – stability of nanoparticles In solutions – synthesis of metal nanomaterials: Physical methods (Laser Ablation, Evaporation, sputtering and solvated metal dispersion) chemical methods (Thermolysis, Sonochemical approach, reduction of metal ions by hydrogen and methanol)

Unit II

Nano material and its applications

Nanotubes – Nanocrystal shape – Sequestration of gases – destructive adsorption of environmental toxins – optical properties – Magnetic properties of nanoscale materials – diamagnetism, paramagnetism, ferromagnetism, and supermagnetism – Size dependent properties such as coercivity (magnetic memory) and saturation magnetization – nanoparticles in polymers, inks fluids, dyes and catalysis – Nanocrystals as colorants, ultraviolet absorbers, electronics – biomedical applications – nano pipettes.

Unit III

Introduction of Green Chemistry

The need for green chemistry – eco efficiency – environmental protection laws, challenges – pollution control and pollution prevention – green

methods, green products, recycling of waste – Twelve principles of green chemistry – inception of green chemistry – awards for green chemistry – international organizations promoting green chemistry.

Unit IV

Solvent Free Organic Synthesis

Solvent free organic synthesis – microwave assisted synthesis – microwave activation, microwave heating – advantages of microwave exposure and specific effects of microwaves – Organic synthesis under microwaves – benefits, limitations, equipments – Reactions on solid supports, phase transfer catalysis, solvent free esters saponification – Reactions without support or catalyst – examples – microwave assisted reactions in water – oxidation of toluene to benzoic acid.

Unit V

Designing Green Synthesis

Green Synthesis – Designing, Choice of starting materials, choice of reagents, choice of catalysts – bio catalysts, polymer supported catalysts, choice of solvents – Synthesis involving basic principles of green chemistry – examples – synthesis of adipic acid, methyl methacrylate, paracetamol – Ultrasound assisted reactions – esterification, reduction, coupling reactions.

References

1. C.P.Poole and F.K.Owens Introduction to Nanotechnology, (2004).
2. T.Pradeep, Nano: The Essential, Tata McGraw Hill Publishing Company Ld., New Delhi, (2008).
3. Mick Wilson, Kamali Kannangara, Geoff smith, Michelle simmons, Burkhard Raguse, 1st Edn., Narinder Kumar Lijhara for overseas Press India Pvt Ltd., New Delhi, (2005).
4. Paul T. Anastas Green Chemistry
5. Sanghi A Shrivastav Green Chemistry.
6. M.Kidwai & Ahlavalia V.K.Green Chemistry
7. V.Kumar, An Introduction to Green Chemistry, Vishal Publishing Co., Jalandhar, 2007.

COMPULSORY PAPER

HUMAN RIGHTS

Paper Code: TUHR20

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
5. Pandey - Constitutional Law.
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.

9. G.S. Bajwa - Human Rights in India.
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.

PRACTICAL-3

ORGANIC CHEMISTRY PRACTICAL – I

Paper Code: TUCH15

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

Any FOUR preparations from the following single stage preparations:

1. Preparation of p-benzoquinone from hydroquinone
2. p-Nitrobenzoic acid from p-nitrotoluene
3. Preparation of 4,6-dimethyl coumarin
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

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.

Conductometric/Potentiometric Titrations- I

1. Conductometric titrations of two components.
 - A. Acid-Base titrations.
 - B. Precipitation titrations.
 - C. Displacement titrations.
2. Conductometric titrations of a mixture of acids (HCl, CH₃COOH) and NaOH.
3. 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.
4. 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
5. Determination of strength of given solution conductometrically by precipitation titration (BaCl₂ vs. MgSO₄).
6. Potentiometric determination of the dissociation constant of weak acid (K_a)
Using quinhydrone/calomel electrode.
7. Potentiometric titrations of a mixture of acids.
8. Determination of solubility product by potentiometry-concentration cell method
9. Potentiometric determination of pH and calculation of pK_a.
10. Determination of strength of KI using potentiometric titration between FAS and KI.
11. Determination of strength of FAS using potentiometric titration between KMnO₄ and FAS.
12. 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, 9th 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.
4. B.P. Levitt (Ed.), Findlay's Practical Physical Chemistry, 9th edn., Longman, London, 1985.
5. 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 **(Organic spectroscopy and Natural Products)**

Paper Code: TUCH31

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 syntheses and uses of natural products*

UNIT-I UV & IR

UV-Visible spectroscopy: Introduction- 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 (Principle only): 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-¹H NMR of simple aliphatic and aromatic compounds.

Principles of ¹³C NMR,- proton decoupled and off – resonance ¹³C NMR spectra – DEPT methods- factors affecting ¹³C chemical shift -¹³C 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 STEROIDS

Occurrence, nomenclature, basic skeleton, Diel's hydrocarbon and stereochemistry of cholesterol. Isolation, structure determination and synthesis of cholesterol, Biosynthesis of Cholesterol.

Conversion of cholesterol into sex hormones such as androsterone, testosterone, estrone and progesterone.

UNIT V ALKALOIDS

Total Synthesis of Alkaloids: Introduction, Sources of alkaloids, Classification, Preussin, Swainsonine, Horsifiline, Ellipticine and Reserpine (Synthesis only)

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, 2nd Edition, 2013.
4. William Kemp, NMR in Chemistry, Mac Millan, 1986.
5. Robert M Silverstein, Francis Webster, Kiemle, Bryce. Spectrometric identification of organic compounds, 8th Ed., Wiley. 2014.

6. Jie Jack Li. E. J. Corey, Total Synthesis of Alkaloids, Springer, 2012.

CORE-8

INORGANIC CHEMISTRY-III

(Solid state and Nuclear Chemistry)

Paper Code: TUCH32

Objectives:

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

- *Basic concepts describing structure of solids and properties of solids.*
- *Basis of nuclear chemistry and types of nuclear reactions*

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-Debye-Scherrer formula-systematic absences, electron and neutron diffraction.

UNIT-II INORGANIC SOLIDS

Ionic bonds- lattice energy of ionic crystals-Born-Haber cycle-Born Lande equation- Madelung constant-Structures-cesium chloride-wurtzite-zinc blende –rutile –fluorite. Defects- types of defects-non –stoichiometry- 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-super conductors.

UNIT-III METAL CLUSTERS

Metal clusters- classification- metal halides and oxides-binuclear clusters-Rhenium dinuclear clusters- structure and bonding-trinuclear clusters, tetranuclear clusters and hexanuclear clusters- Chevrel phases- Wade's rule-polyatomic zintl anions and cations (naked clusters).

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, GM and Scintillation counters. Nuclear Reactions: Types, reactions, cross section, Q-value, nuclear fission and fusion reactions as energy sources; direct reactions; photonuclear and thermo nuclear reactions.

- *To understand and appreciate the quantum mechanical approach to the atomic and molecular electronic structure.*
- *To learn the applications of photochemistry.*
- *To learn the principles and applications of statistical thermodynamics 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.*

UNIT-I ELECTROCHEMISTRY-I

Electrochemistry of solutions: Ionic atmosphere, Kohlrausch law and its applications-Debye-Huckel-Onsager equation-Derivation-validity and deviation -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 and its significance-Butler-Volmer equation (single step, one electron transfer only) - Exchange current density. Nernst equation as a special case of Butler-Volmer equation-Reaction resistance-Polarisable and non-polarisable electrodes-Low and high field approximations-Tafel equation.

Fuel cells-Classification-Chemistry of fuel cells-detailed description-Ion-selective electrodes.

Polarography: Residual current-limiting current-Ilkovic equation, half wave potential and its significance, polarographic maxima-qualitative and quantitative estimation of metal ions.

UNIT-III QUANTUM CHEMISTRY-II

Applications of wave mechanics- Harmonic oscillator- Rigid rotator-Hydrogen atom solution (No derivation required).

Approximation methods-Variation method, Perturbation method for non-degenerate and time-independent system-Slater determinant-Anti-symmetric wavefunctions-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-IV STATISTICAL THERMODYNAMICS

Objectives of statistical thermodynamics, Concept of distributions, Types of ensembles. Thermodynamic probability, Most probable distribution Law-Classical statistics-Maxwell-Boltzmann (MB) statistics-Quantum statistics-Bose-Einstein (BE) and Fermi-Dirac (FD) statistics-Derivation of distribution function-MB, BE and FD statistics comparison-Partition functions-Translational, rotational, vibrational and electronic partition function (Problem only)- Relation between entropy and partition function; Debye and Einstein heat capacity of solids. Ortho and para hydrogen.

UNIT-V PHOTOCHEMISTRY

Franck-Condon principle-Jablonskii diagram-primary and secondary processes-Flourescence and phosphorescence-Quantum yield-Chemical actionometry-Photosensitization, chemiluminescence.

Kinetics of photochemical processes-H₂ and Cl₂ reaction-Excimers and Exciplexes. Mechanism of fluorescence quenching- Stern-Volmer equation and its applications. Photodegradation of polymers-Atmospheric photochemistry.

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.K. Prasad, Quantum chemistry, Wiley Eastern, 1993.
6. W. Levine, Quantum chemistry, Prentice-Hall, 2000.
7. Donald A.McQuarrie, Quantum chemistry, University science books, Oxford University Press, 1983 .

8. Thomas Engel and Philip Reid, Thermodynamics: Statistical thermodynamics and Kinetics, Pearson, 2012.
9. M.C. Gupta, Statistical thermodynamics, New Age International, Pvt., Ltd., New Delhi, 1995.
10. F.W. Sears, G.L. SalingerTurcotte; Statistical thermodynamics, Narosa Publishing house New Delhi, 1998.
11. N.J.Turro, Modern Molecular Photochemistry, Benjamin, Cumming, MenloPark, California.
12. K.K.Rohatgi, Mukherjee, Fundamentals of Photochemistry, New Age International Pvt. Ltd, Chennai, 2009.
13. R.P.Wayne, Photochemistry, Butterworths, London.

ELECTIVE-3A GREEN AND INDUSTRIAL CHEMISTRY

Paper Code: TUCH34A

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 make the students knowledgeable in solar energy conversion.*
- *To understand the basics of water chemistry.*
- *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 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-III WATER TREATMENT

Sources of water – Quality characteristics of water: total acidity and alkalinity, hardness of water – methods of determination of hardness, total solids, disadvantages of using hard water.

Softening of water: Desalination, Clark's process, lime-soda process, ion-exchange process; demineralization of water - Treatment of water: sterilization, flocculation, Industrial treatment – Treatment of wastes or effluents with organic and inorganic impurities, sewage and sewage treatment; Biochemical oxygen demand (BOD), chemical oxygen demand (COD)

UNIT IV: PLASTICS

Thermosetting and thermoplastics- Effect of polymer structure on properties.

Formation of plastics: copolymerization-properties and uses of plastics- Manufacture by molding process-Commercial resins and plastics: bakelite, urea-formaldehyde, melamine-formaldehyde, epoxy, acrylic and silicon resins, polythene, PVA, PVC, cellulose, cellulose nitrate and acetate.

Disposing of plastics: incineration, biodegradation, recycling and source reduction.

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).
6. Engineering Chemistry- Jain and Jain.
 7. Engineering Chemistry- R.K. Sharma.

ELECTIVE-3B SURFACE ANALYTICAL TECHNIQUES & SENSORS

Paper Code: TUCH34B

Objectives:

After this course the student should be able

- *To understand the principles of ESCA, 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.*

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, adulterants, 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 Vikerma, 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.

ELECTIVE-3C COMPUTATIONAL METHODS IN CHEMISTRY AND CHEMOMETRICS

Paper Code: TUCH34C

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.*

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 discriminant analysis, Modeling 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, 6th Edition, 2010.

4. Brereton, R.G, Chemometrics: Data Analysis for the Laboratory and Chemical Part, Wiley, 2003.

OPEN ELECTIVE -2OE1 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.*

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 - chlorofluorocarbons and their interactions with ozone – the Antarctic 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), (10th Edition),
2. M.Gopala Rao, Outlines of Chemical Technology – For the 21st Century – & Marshall Sittig, 3rd Edition.
3. Bailey, Clark, Ferris, Isrause, Strong, Chemistry of the environment, 2nd 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

OPEN ELECTIVE – 2OE2 RADIATION CHEMISTRY AND SPECTROSCOPY

Objectives:

- *The students should be able to know the about nuclar chemistry and radioativity.*
- *This paper enables a student to understand the isotopes, radiation measurements and units*
- *Non major students should be able to unbdertstand the basic principles of variousradiation analysis.*
- *The students should be able to understand the advanced optical spectroscopic techniques and interaction of radiation with matter.*

UNIT-II Radiation Chemistry-1

Elements of radiation chemistry – Radiation chemistry, passage of nucleous through matter, interaction of radiation with matter, Units. for measuring radiation absorption, Radiation dosimetry, Radiolsis of water, free radiation in water Radiolsis, Radiolysis of some aqueous solution.

UNIT-III Radiation Chemistry -2

Radio Chemistry : recapitulation – type of radioactive decay, Detection & measurement of radiation (G.M. & Scintillation counter) Applications of radioactivity : General principles of using radioisotopes. - Physical constants – Diffusion coefficients, surface area, solubility. - Analytical applications- neutron activation analysis, dilution analysis, radiometric titration. Industrial applications.

Unit III Nuclear Reactors

The fission energy, The Natural uranium reactor, the four factor formula- The reproduction factor K, the classification of reactor. Reactor power, Critical size of thermal reactor, excess reactivity & control, the Breeder reactor, The Indians nuclear energy programme, Reprocessing of spent fuel : Recovery of Uranium & Plutonium, Nuclear waste management, Natural nuclear reactor.

UNIT-IV 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.

Unit-V 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.

Reference books

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

Open Elective 2OE3 CHEMISTRY OF BIOMOLECULES

Objectives:

- *The non-chemistry students should be able to know the chemical nature of the bioproducts.*
- *This paper enables a student to understand the basic chemical structure and their properties of plant and other bioproducts*
- *The students should be able to understand the isolation and structural elucidation of natural products.*

UNIT-I Chemistry of plant products

Anthocyanins: Methods of isolation, basic structural features of coumarins, chromones, flavones and isoflavones. Structural elucidation of quercetin and wedelactone (synthesis not included). Carotenoids: Methods of isolation; Structure elucidation of b-carotene; structural relationship of α , β and γ -carotenes.

Unit II Lipids

Introduction, isolation and properties of lipids. Oils and fats: definitions and significances of hydrogenation, iodine value, saponification value and auto-oxidation of oils and fats. Phospholipids: lecithins, cephalins and phosphatidyl serine. Sphingolipids: sphingosine, sphingomyelin and cerebrocides.

UNIT-III Terpenoids:

Introduction, Biological importance, Nomenclature, Occurance and isolation; Isoprene rule; Structure and biosynthesis of monoterpenoids, sesquiterpenoids, diterpenoids and triterpenoids; Structures of camphene, pinenes, camphor, borneols.

Unit IV Steroids:

Sterols and Bile acids; Nomenclature, Basic skeleton, Diels hydrocarbon. Isolation, structure and structures of sterols and bile acids, stereochemistry at ring junctions. Structure and biological significance of Estrone, Progesterone, androsterone, testosterone; Photoproducts of ergosterol-vitamins D.

Unit V Carbohydrates

Types of naturally occurring sugars. Deoxy sugars, amino sugars, branched chain sugars, methyl ethers and acid derivatives of sugars. General methods of structure and ring size determination with particular reference to maltose, lactose and sucrose. Structure, degradation and biological functions of starch, cellulose and chitin.

SUGGESTED BOOKS

1. Biochemistry, J. David Rawn, Neil Pattuson publishers, North Carolina, (USA) 1989.
2. Organic Chemistry. Vol I and Vol II, I. L. Finar, 6th edn. ELBS & Longman (London), 1975.
3. Introduction to Lipids, D. Chapman, McGraw-Hill, 1969.
4. Advanced general Organic Chemistry, S. K. Ghosh, DK and Allied publishers (UBS), Calcutta, 1998.
5. Text book o Biochemistry, E. S. West, W. R. Todd, H. S. Mason & J. T. Van Bugen, 4th Edn. Amerind publishing co. (New Delhi), 1974.

PRACTICAL-5

ORGANIC CHEMISTRY PRACTICAL- II

Paper Code: TUCH35

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 oil
Estimation of sulphur in an organic compound
Estimation of methyl ketone

Special Interpretation Of Organic Compounds- IR, NMR and MASS Spectra of the following types of compounds

1. Alcohls (primary, secondary and tertiary)
2. Aldehydes
3. Ketones
4. Mono&dihalo compounds
5. Amines
6. Esters
7. Amides
8. Alkenes and alkynes

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. Preparation of 2,4,6-tribromiodobenzene
5. m-Nitro benzoic acid from benzaldehyde
6. Preparation of p-nitroacetanilde
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

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.

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.
5. N.S. Gnanapragasam and B. Ramamoorthy, "Organic Chemistry Lab Manual" (2006), S. Visvanathan Printers & Publishers.

PRACTICAL-6 INORGANIC CHEMISTRY PRACTICAL – II

Paper Code: TUCH36

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 ClF_3

^1H NMR Spectra of Tris (ethylthioacetanato) cobalt (III)

Explain high resolution ^1H NMR spectra of (N-propylisonitrosoacetylacetonate) (acetylacetonate) Nickel (II)

ESR Spectra of the aqueous $\text{ON}(\text{SO}_3)^{2-}$ ion.

ESR Spectra of the H atoms in CaF_2 .

ESR Spectra of the $[\text{Mn}(\text{H}_2\text{O})_6]^{2+}$.

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 $\text{FeSO}_4 \cdot 7\text{H}_2\text{O}$

Mossbauer spectra of FeCl_3 .

Mossbauer spectra of $[\text{Fe}(\text{CN})_6]^{3-}$

Mossbauer spectra of $[\text{Fe}(\text{CN})_6]^{4-}$

Reference

Vogel's Textbook of Quantitative Chemical Analysis, 6th Edition

SEMESTER-IV

CORE-10

ORGANIC CHEMISTRY –IV (ADVANCED ORGANIC CHEMISTRY)

Paper Code: TUCH41

Objectives:

- *To learn various organic reactions and reagents used in them as tools applied in the art of organic synthesis. To learn retrosynthetic approach towards organic synthesis.*
- *At the end of the course, the learners should be able to use various reagents and organic reactions in a logical manner in organic synthesis.*
- *Learnt the basic principles of photochemistry and pericyclic reactions*

UNIT-I SYNTHETIC METHODOLOGY

An introduction to synthons and synthetic equivalents, functional group interconversions, Planning and execution of multistep synthesis- overall 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 polarity, cyclization reactions, amine synthesis.

UNIT-II MODERN SYNTHETIC METHODS

Modern Synthetic Methods: Baylis-Hillman reaction, Kulinkovich reaction, Ritter reaction, Sakurai reaction, Brook rearrangement. Palladium mediated C-C and C-X coupling reactions: Heck, Stille, Suzuki, Negishi and Sonogashira coupling reactions. Stereoselective synthesis of tri- and tetra-substituted olefins, Synthetic applications of Claisen rearrangement.

UNIT-III CONSTRUCTION OF RING SYSTEMS

Construction of Ring Systems: Different approaches towards the synthesis of three, four, five, and six-membered rings. Pauson-Khand reaction, Bergman cyclization; Nazarov cyclization, inter-conversion of ring systems (contraction and expansion). Construction of macrocyclic rings and ring closing metathesis.

UNIT-IV PHOTOCHEMISTRY

Organic photochemistry – fundamental concepts –Joblonski diagram -energy transfer –characteristics of photoreactions – photoreduction and photooxidation, photosensitization. Photoreactions of ketones and enones – Norrish Type I and II reactions – Paterno-Buchi reaction – photo-Fries rearrangement – photochemistry of alkenes, dienes and aromatic compounds – di- π -methane rearrangement. Photochemistry of α,β -unsaturated carbonyl compounds – photolytic cycloadditions and photolytic rearrangements – photo additions – Barton reaction.

UNIT- V PERICYCLIC REACTIONS

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 rotatory 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. R.O.C. Norman, Principles of Organic Synthesis, Second edn., Chapman and Hall, 1993.
2. R.K. Mackie, D. M.Smith and R.A. Aatkin, Guide Book to Organic Synthesis, 2ndedn. Longman Scientific and Technical, London, 1990
3. S.Warren, Designing Organic Synthesis – A Programmed Introduction to Synthon Approach, Wiley, NY, 1978
4. R.O.C. Norman, Principles of Organic Synthesis, II Edn., Chapman and Hall, 1993.
5. Jaya singh and Jagadhambasingh, Photochemistry and Pericyclic reactions, New Age international Publishers, New Delhi, 2010.
6. N.J.Turro, Modern Molecular Photochemistry, Benjamin, Cumming, Menlo Park, California.
7. K.K.Rohatgi, Mukherjee, Fundamentals of Photochemistry, New Age International Pvt. Ltd, Chennai, 2009.
8. R.P.Wayne, Photochemistry, Butterworths, London.

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 information 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: Mission and history-CA weekly issues, CA issue indexes. Retrospective 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).

UNIT-IV SCIENTIFIC WRITING

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

UNIT-V COMPUTER SEARCHES OF LITERATURE

ASAP Alerts, CA Alerts, SciFinder, ChemPort, ScienceDirect, Web of science, Scopus, STN International.

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.

ELECTIVE-4A APPLICATION OF SPECTRAL TECHNIQUES TO INORGANIC COMPOUNDS

Paper Code: TUCH43A

Objective:

- *On the completion the course the students will have the knowledge of applications of various spectral techniques to inorganic compounds.*

UNIT-I ELECTRONIC SPECTROSCOPY

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.

UNIT-II INFRARED AND RAMAN SPECTROSCOPY

IR spectroscopy-principle-fundamental modes of vibrations- H_2O , CO_2 and SO_2 -change of IR spectra of ligands upon coordination-urea, thio urea, SO_4^{2-} , NO_3^- , nitriles, carboxylate, cyanate and thiocyanate anions. Finger

print region- IR spectra of metal carbonyls. Effect of isotopic substitution on IR spectra.

Raman spectroscopy-principle-mutual exclusion principle-combined application of IR and Raman to inorganic molecules.

UNIT-III NMR SPECTROSCOPY

Application of NMR (^{19}F , ^{31}P and ^{13}C) techniques to characterize the inorganic compounds. Chemical shifts-application of spin-spin coupling to structure determination- H_3PO_3 and H_3PO_2 , P_4 S_3 , BrF_5 , - applications involving magnitude of coupling constants-consequences of nuclei with quadrupole moments-NMR shifts of paramagnetic complexes-Contact shifts-spectrum of $\text{P}_3\text{N}_3\text{Cl}_4\text{F}_2$, $\text{P}_4\text{N}_4\text{Cl}_6$.

UNIT-IV 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.

UNIT-V MOSSBAUER SPECTROSCOPY

Principle-Isomer shifts - Magnetic interactions - Mossbauer emission spectroscopy - application to low and high spin iron and tin compounds.

Reference Books

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

ELECTIVE-4B INSTRUMENTAL METHODS OF ANALYSIS

Paper Code: TUCH43B

Objectives:

On the completion the course the students will have the knowledge of

- *Various instrumental techniques.*
- *The students should have learnt data analysis and electroanalytical 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

Paper Code: TUCH43C

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.

CORE-12

PROJECT

Paper Code: TUCH44

Field of Project – Organic / Inorganic / Physical Chemistry

No. of hours/week : 18

No. of Credit : 05

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

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Chapter No.	TITLE
1.	Introduction
2.	Review of Literature
3.	Materials and Methods
4.	Results and Discussion
5.	Summary
6.	References
