



**NOTIFICATION**

Sub: Revised syllabus of M.Sc. in Industrial Chemistry programme.

Ref: Academic Council approval vide agenda

No.: ಎಸಿಸಿ:ಶೈ.ಸಾ.ಸ.3:101 (2021-22) dtd 17.12.2021.

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The Revised syllabus of M.Sc. Industrial Chemistry programme which is approved by the Academic Council at its meeting held on 17.12.2021 is hereby notified for implementation with effect from the academic year 2021-22.

Copy of the Syllabus shall be downloaded from the University Website ([www.mangaloreuniversity.ac.in](http://www.mangaloreuniversity.ac.in))

  
REGISTRAR

To,

1. The Chairman, Dept. of Industrial Chemistry, Mangalore University, Mangalagangothri
2. The Chairman PG BOS in Industrial Chemistry, Dept. of Industrials Chemistry Mangalore University.
3. The Registrar (Evaluation), Mangalore University.
4. The Superintendent (ACC), O/o the Registrar, Mangalore University.
5. The Asst. Registrar (ACC), O/o the Registrar, Mangalore University.
6. Guard File.

**MANGALORE UNIVERSITY**  
**DEPARTMENT OF INDUSTRIAL CHEMISTRY**

**M. Sc. DEGREE PROGRAMME IN INDUSTRIAL CHEMISTRY**

(Effective from the Academic Year 2021-22)

**Two years Master Degree programme (Four Semesters) M.Sc. Industrial Chemistry (CBCS)**

**PREAMBLE**

Revision of syllabi for the two years' Master Degree (Choice Based Credit System- Semester Scheme) Programme in Industrial Chemistry

PG BOS in Industrial Chemistry has revised and prepared the syllabi (CBCS based) for the PG course in Industrial Chemistry by giving certain guidelines to offer Hard Core, Soft Core and Open Elective courses with credits to each course amounting to **90** credits for the entire programme.

There are totally **9** theory courses, One semester Industrial project in IV semester are assigned as Hard Core courses with a total credits of 54. Students have to study 3 soft core courses each in I ,II and III semester. The choice has been given for the soft core courses in the I ,II and III semesters for Industrial chemistry post graduates. All 9 practical courses will be taught as soft courses with 2 credits for each courses in I and II semester where as III semester practical courses are given 3 credits. Total Soft core credits amount to 30. Board of Studies in Industrial chemistry has carefully chosen two Open Elective courses for the students from other disciplines, one each in II and III semester, with total credits of 6. Therefore, grand total credits for the programme = **90**.

A detailed skeleton of the entire programme is being tabulated for the benefit of the aspiring post graduates. Other important aspects such as University question paper pattern, internal assessment examinations, allotment of marks and the approximate dates of the internal examinations are being tabulated with a discussion in the BOS.

**Program Objectives:**

The M.Sc. Industrial chemistry course has an objective to impart knowledge of chemistry and hands-on experience to the students. The program includes an in-depth study on a number of areas in chemical sciences to which students are introduced at the core curriculum level, theoretical and experimental solutions to various problems and molding the students relevant to contemporary industries. The areas introduced by the department include agrochemicals, pharmaceutical chemistry and Petrochemicals. Beside the theoretical and laboratory based curriculum, students complete an advanced project in the final semester of the program at an industry.

The degree provides a solid foundation in the discipline of core chemical sciences, critical thinking and problem solving skills. During the academic program students also develop excellent written and oral communication skills, learn to work as a team and project management.

**The objectives of this Postgraduate program include:**

- To provide the highest level of education in chemical sciences and provide competent, creative and imaginative scholars.
- To encourage free will and objective oriented enquiry for knowledge.
- To make a significant contribution towards the development of skilled technical manpower. Thus cater to the need of growing demand of intellectual reservoir in the nation.
- The program is designed to achieve the objectives and to inculcate in the students concepts and intellectual skills, courage, integrity, awareness and sensitivity towards the needs and aspirations of the society.

**Two-year Master's Degree Course  
(Four Semesters) M Sc Industrial  
Chemistry (CBCS)**

Sl. No.	Semester	Hard core credits	Soft core credits	Open elective credits	No. of Practical Paper Project*	No. of Theory Paper	Total credits
1.	I Semester	12	9	-	3 (S)	3(H) +1(S)	21
2.	II Semester	12	9	3	3 (S)	3(H)+1(S)	24
3.	III Semester	12	12	3	3(S)	3(H)+1(S)	27
4.	IV Semester	18	---	--	Industrial Project (H)	-----	18
	<b>Total</b>	<b>54</b>	<b>30</b>	<b>6</b>			<b>90</b>

Description of course	Courses Hard Core/ Soft core	Teaching Hrs/week	Credits	Hrs. of exam	Max Marks: Exam + IA = Total
<b>I SEMESTER</b>					
ICH 401 : Inorganic Chemistry	H	4	4	3	70+30=100
ICH 402 : Organic Chemistry-I	H	4	4	3	70+30=100
ICH 403 : Physical Chemistry	H	4	4	3	70+30=100
ICS 404: Environment Health and Safety Measures	S	3	3	3	70+30=100
ICS 405: Paper and Textile technology	S				
ICP406 : Inorganic Chemistry Practicals-I	S	4	2	4	70+30=100
ICP 407 : Organic Chemistry Practicals-I	S	4	2	4	70+30=100
ICP 408 : Physical Chemistry Practicals-I	S	4	2	4	70+30=100
			<b>21</b>		<b>700</b>
<b>II SEMESTER</b>					
ICH451 : Analytical Chemistry	H	4	4	3	70+30=100
ICH452 : Advanced organic Chemistry	H	4	4	3	70+30=100
ICH453:Energy Systems, Colloids and Petrochemicals	H	4	4	3	70+30=100
ICS 454 : Chemical Engineering Technology	S	3	3	3	70+30=100
ICS 455: : Chemical analysis in agro and food industries	S				
ICP 456 : Techniques in quantitative analysis	S	4	2	4	70+30=100
ICP 457 : Estimations and extractions in organic chemistry	S	4	2	4	70+30=100
ICP 458 : Electroanalytical techniques	S	4	2	4	70+30=100
ICE 459 : Industrial Safety, Environmental and Electrochemical Sciences	OE	3	3	2	70+30=100
			24		<b>800</b>
<b>III SEMESTER</b>					
ICH 501 : Spectroscopic Techniques	H	4	4		70+30=100
ICH 502 : Industrial Catalysis and polymers	H	4	4	3	70+30=100
ICH 503: Synthetic, Heterocyclic and Medicinal Chemistry	H	4	4	3	70+30=100
ICS 504: Polymers and Soft materials	S	3	3	3	70+30=100
ICS 505: Computer aided drug design	S				
ICP 506: Synthesis of complexes, catalysts and estimation of alloys	S	6	3	5	70+30=100
ICP 507: Systematic qualitative analysis and identification of organic compounds	S	6	3	5	70+30=100
ICP 508: Synthesis, characterization and applications of Polymers and composites	S	6	3	5	70+30=100
ICE 509: Agriculture and Health care Chemicals	OE		3	2	70+30=100
			<b>27</b>		<b>800</b>
<b>IV SEMESTER</b>					
Project Work (4 Months ) ICH 551 : Project Report ICH 552 : Viva-voce Examination	H		<b>18</b>		400+200 100
					<b>Total= 700</b>
			<b>90</b>		<b>Grand Total=3000</b>

## **BASIS FOR INTERNAL ASSESSMENT**

Internal assessment marks in theory papers of I, II and III semesters shall be based on average of two tests conducted 10<sup>th</sup> and 14<sup>th</sup> weeks after the start of a semester.

- Internal assessment in I Semester shall be awarded as: 20 marks for Test and 10 marks for assignment written on a given industrially related topic.
- Internal assessment in II Semester shall be awarded as: 20 marks for Test and 10 marks for seminar for hard core subjects and assignment for softcore subjects.
- Internal assessment in III Semester shall be awarded as: 20 marks for Test and 40 marks for industrial visit report which will be equally distributed to three hard core and one soft core paper.
- Practical internal assessment marks shall be based on test (25) and record (5) for I semester. For II and III semesters IA shall be based on practical test (15 marks), Viva (10 marks) and record (5marks). The practical test may be conducted towards the end of the semester.

## **THEORY QUESTION PAPER PATTERN FOR HARD CORE, SOFT CORE AND OPEN ELECTIVE COURSES**

### **Question Papers in all the four semesters shall consist of Parts A and B.**

- **Part A** shall contain eight (8) very short answer objective type questions carrying 2 marks each drawn from all the four units of the syllabus (2 questions per unit). Five (5) questions are to be answered. There may be a maximum of two sub-divisions per question, carrying one (1) mark per sub-division.
- **Part B** shall contain eight (8) brief and/or long answer questions carrying 12 marks each drawn from all the units of the syllabus (minimum 2 questions per unit). There may be a maximum of three sub-divisions per question, carrying 3 or more marks per sub-division. Five (5) out of eight (8) questions are to be answered from Part B.

## **PRACTICALS EXAMINATION PATTERN**

In the I semester 70 marks shall be awarded based on the experiment. But in the II and III semesters, out of 70 marks, 20 marks are for the viva-voce to be conducted during practical and 50 marks for the experiment and the scheme of evaluation can be decided by the examiners during examination.

Candidates of IV semester shall undergo a compulsory project work in an industry for four months and prepare a report on their work. The Project Report shall be evaluated by two examiners as in the case of theory papers. Internal Assessment marks shall be allotted by project supervisors at the Industry. The progress of the project work of a student will be evaluated time to time by internal guide from the department. Viva-Voce examination is to be conducted as per the University regulations.

# I SEMESTER

## ICH 401: INORGANIC CHEMISTRY

### Course objectives:

- To learn the basic concepts and theories involved in Coordination Chemistry
- To understand the significance and to explain the applications of coordination complexes.
- To learn different metallurgical process.
- To know diverse organometallic compounds and their reactions.
- To understand the symmetry and transitions of molecules.

### UNIT I:

14 hr

**Coordination Chemistry:** Introduction and important terms pertaining to coordination compounds and naming of coordination compounds, Isomerism in coordination compounds (types of stereo isomerism and structural isomerism examples), theories of coordination chemistry : postulates and defects of Werner's theory, Sidgwick's electronic concept theory (Effective Atomic Number Rule), Valence bond theory, Crystal field theory (crystal field splitting in octahedral and tetrahedral coordination entities), Molecular orbital theory of coordination complexes, thermodynamic and kinetic stability, magnetic properties, colours of coordination compounds, factors affecting the stability of coordination compounds, significance and applications.

### UNIT II:

14 hr

**Organometallics:** Historical development, classification and nomenclature, stability, 16 and 18 electron rules, Transition metal alkyls and aryls- types, routes of synthesis, stability and decomposition pathways, Nucleophilic and electrophilic cleavage of metal-carbon sigma bonded compounds. Alkane activation. Transition metal to carbon multiple-bonded compounds-carbonyls, nitrosyls, metal-alkene, metal cyclopentadiene, metal-arene complexes.

### UNIT III:

14 hr

#### **Bioinorganic Chemistry**

Transport and storage of dioxygen- heme proteins, oxygen uptake, functions of haemoglobin, myoglobin, hemerythrin and hemocyanins, synthetic oxygen carriers. Metal storage and transport – ferritin, transferrin and ceruloplasmin. Electron transfer proteins-cytochromes, iron-sulphur proteins. Metalloproteins as enzymes-carboxy peptidase, carbonic anhydrase, alcohol dehydrogenase, catalases, peroxidases, cytochrome P450, superoxide dismutase, copper oxidases, vitamin B12 coenzyme.

### UNIT IV:

14 hr

**Molecular Symmetry and Group Theory:** Symmetry elements and operations, Group theory- Concept of a group, definition of point group. Classification of molecules, Group multiplication tables. Matrix representations of symmetry operations, class similarity transformation, reducible and irreducible representations. The great orthogonality theorem. Character tables, relationship between representations and wave functions. Group theory and hybrid orbitals. Group theory and MO's. Molecular vibrations- Symmetry types of normal modes of vibrations. Selection rules for fundamental vibrational transitions, symmetry considerations to determine IR active and Raman active lines.

### Course Outcome:

The students would be learning

- The nature of bonding in coordination compounds in terms of the valence bond and crystal field theories; and the stability of coordination compounds
- Account for the importance and applications of coordination compounds in our day to day life.
- Principles and applications of organometallic chemistry
- Metallurgical process used in industries to extract metals and related applications.
- Molecular symmetry and group theory to understand structure and spectroscopy.

### References

1. Carter Robert I: Molecular Symmetry And Group Theory, John Wiley,2005
2. Agarwala U C Et Al., Molecular Symmetry In Chemistry Via Group Theory, Ane Books, 2013.
3. V. Ramakrishnan And M.S. Gopinathan: Group Theory In Chemistry, Vishal,1988
4. Heine, Volker: Group Theory In Quantum Mechanics An Introduction To Its Present Usage, Pergamon, 1964.
5. F.A. Cotton: Chemical Applications of Group theory, Wiley, New York,1993.
6. Bodsworth C: Metallurgy and metallurgical engineering series,CBS,1988
7. Johnson, Carl G :Metallurgy , The times of india,1956.
8. Chemistry of the Elements, N.N.Greenwood & A. Earnshaw, Butterman-Helmman, 2005.
9. Principles of Extractive Metallurgy, H. S. Ray and A. Ghosh.
10. Extraction of Nonferrous Metals, H. S. Ray, R. Shridhar and K. P. Abraham.
11. Gilchrist, J. D, Extraction metallurgy, Pergamon, 1989.
12. Organometallic Chemistry, R.C.Mehrotra and A.Singh, New Age International, 1999.
13. Advanced Inorganic Chemistry, F.A.Cotton and G.Wilkinson, Wiley, 1991.
14. Concise Inorganic Chemistry, J.D. Lee, Fifth edition,2008.
15. Advanced Inorganic Chemistry, Gurdeep Raj Vol I and Vol II First edition 2019.
16. Textbook of Inorganic Chemistry, G.S Sodhi. First edition 2013.
17. Inorganic Chemistry, J.E. Huheey, E.A. Keiter, and R.L Keiter, 4th Ed.1993.

## ICH 402: ORGANIC CHEMISTRY

### Course objective

- To study the acid base concept in organic chemistry
- To know the nature of reaction intermediates and the factors affecting reaction conditions such as nature of solvent, isotope effects and salt effects.
- To learn about reaction types and their kinetics, thermodynamic and effect of thermodynamic parameters on reaction with kinetic aspects.
- To understand aliphatic and aromatic nucleophilic and electrophilic substitution by studying their mechanism with factors effecting and related named reactions.
- To discover various aspects of stereochemistry and applications of chirotechnology.

#### UNIT I:

14 hr

**Reaction intermediates:** Generation, structure, stability, reactivity & detection of classical & non-classical carbocations, carbanions, free radicals, carbenes, nitrenes & arynes. N, S & P ylides & enamines.

**Organic Reactions and Mechanism:** Reaction mechanism & types, types of organic reactions, reaction profile diagrams, thermodynamic & kinetic control, leaving group and solvent. Methods of determining reaction mechanisms: Kinetic & non-kinetic methods-identification of products, detection of intermediates, isotopic labelling, stereochemical evidences, cross-over experiments, kinetic evidences & kinetic isotopic effects. The Hammond postulate. Principle of microscopic reversibility and Marcus theory. **Acids and Bases:** Introduction to acids and bases, Bronsted-lowry and acid-bases concept, organic acids and bases, pKa and pH, effect of solvent on acid and base strength, effect of structure of organic compound on acid and base strength. Reactivity in relation to molecular structure and conformation. Steric effects. F strain, B-strain. Bond angle strain. The Hammett equation and its applications, Ortho effect. Taft equation. Linear free energy relationships

#### UNIT II: Organic Reactions and Mechanism (Part-I)

14 hr

**Aliphatic Nucleophilic Substitution reactions:** Mechanisms Nucleophilic substitution: Substitution reactions of ambident nucleophiles, neighbouring group participation of O, S, N, halogens, aryl groups, alkyl and cycloalkyl groups in nucleophilic substitution reactions. Sigma, Pi bond participation in acyclic and bicyclic systems (Non-classic carbocations) Substitution at allylic, trigonal and Vinylic carbons, Meyer's synthesis of aldehydes, ketones and carboxylic acids, alkylation with trialkyl boranes. **Aliphatic Electrophilic substitutions:** SE1 SE2 and SEi mechanisms hydrogen exchange, migration of double bonds, halogenation of aldehydes, ketones, acids, acylhalides sulphoxides and sulphones, aliphatic diazonium coupling, nitrosation at carbon and nitrogen diazo transfer reaction. Decarboxylation of aliphatic acids. Haloform reaction and Haller-Bauer reaction.

#### UNIT III: Organic Reactions and Mechanism (Part-II)

14 hr

**Aromatic nucleophilic substitution:** A general introduction to different mechanisms of aromatic substitution SN Ar, AN and aryne, Von Richter rearrangement, Sommet, Hauser rearrangement Smiles rearrangement. Radical substitution Mechanism: Reaction at sp<sup>3</sup> carbon: Reactivity in aliphatic substrates reactivity at bridged position, reactivity at sp<sup>2</sup> carbon. Reactivity in aromatic substrates neighbouring group assistance in free radical reactions, effect of reactivity in the attacking radical, effect of solvent on reactivity halogenation at an alkyl carbon and allylic carbon, hydroxylation at aromatic carbon by means of Fenton's reagent, oxidation of aldehydes to carboxylic acids, formation of cyclic ethers with Pb(OAc)<sub>4</sub> Reed reaction, Sandmeyer reaction, Kolbe reaction and Hunsdiecker reaction.

**Addition Elimination Mechanisms:** (a) Addition to carbon multiple bonds- Addition reactions involving electrophiles, nucleophiles and free radicals, cyclic mechanisms, orientation and stereochemistry, hydrogenation of double and triple bonds, hydroboration, Birch reduction. Michael reaction, (b) Addition to carbon-hetero atom multiple bonds: Mannich reaction AH reductions of Carbonyl compounds acids, esters, nitrites, addition of Grignard reagents, Reformatsky reaction, Tollen's reaction, Wittig reaction, Prins reaction: (c) Elimination reactions:



Stereochemistry of eliminations in acyclic and cyclic systems, orientation in eliminations - Saytzeff and Hoffman elimination propolitic elimination.

#### UNIT IV: Stereochemistry

14 hr

Concept of chirality, optical isomerism, D,L-; R,S- designations, geometrical isomerism and E,Z designations, Stereoselective and stereospecific reactions, Racemisation, mechanism of racemisation, resolution of racemic mixtures, Asymmetric synthesis-definition, importance, mechanism, energy consideration, advantages and limitations, methods of determination of enantiomeric excess. Enantioselective reactions, The chiral pool, chiral auxiliaries and chiral reagents. Use of  $\alpha$ -amino acids in the synthesis of benzodiazepines, carbohydrates in the synthesis of swainsonine (D-mannose) and timolal (mannitol). Synthesis and applications of oxazaborolidines,  $\text{IPC}_2\text{BH}$ , (S)-BINAP-DIAMINE and (R)-BINAL-H.

#### Course outcome

- The student would understand the acid base concept in organic chemistry and would know the nature of reaction intermediates and the factors affecting reaction conditions such as nature of solvent, isotope effects and salt effects
- The kinetics and energetics of  $\text{S}_{\text{N}}2$ ,  $\text{S}_{\text{N}}1$ ,  $\text{S}_{\text{N}}\text{i}$ ,  $\text{S}_{\text{E}}1$ ,  $\text{S}_{\text{E}}2$ ,  $\text{S}_{\text{E}}\text{i}$ , aromatic nucleophilic and electrophilic substitution by understanding their mechanisms with factors effecting and related named reactions would be understood by the student .
- Basic concept of stereochemistry and applications of stereochemistry would be learnt by studying asymmetric synthesis and use of chiral reagents.

#### References:

1. Robert B. Grossman :The Art of Writing Reasonable Organic Reaction Mechanisms  
Second Edition, © 2003, Springer-Verlag New York, Inc. 1999.
2. Daniel E. Levy: Arrow Pushing in Organic Chemistry An Easy Approach to Understanding Reaction Mechanisms John Wiley & Sons, Inc., Hoboken, New Jersey, 2008.
3. Audrey Miller, Philippa H. Solomon: Writing Reaction Mechanisms in Organic Chemistry, Elsevier Science & Technology Books, ISBN: 0124967124, 1999
4. Organic Chemistry-P.Y.Bruice (Pearson Education Pvt. Ltd., New Delhi),2002.
5. Advanced Organic Chemistry-Reactions, mechanisms & structure-J.March (Wiley, NY)2000.
6. Organic Chemistry-Vol. -1,2 &3- Mukherji, Singh and Kapoor. (Wiley Eastern,) 1994.
7. A guide book of mechanisms in Organic Chemistry-P.Sykes (Orient- Longman) 1985.
8. Organic Chemistry-R.T. Morrison and R.N. Boyd (Prentice Hall, New Delhi) 1994.
9. Organic Chemistry 4<sup>th</sup> Edn.-S.H. Pine et al (McGraw-Hill, London) 1987.
10. Advanced Organic Chemistry- R.A. Carey and R.J. Sundberg (Plenum, New York)1990.
11. Modern Concepts of Advanced Organic Chemistry-R.P. Narein (Vikas, Delhi) 1997.
12. A Text book of Organic Chemistry-Tewari, Vishnoi and Mehrotra (Vikas, New Delhi)1998.
13. A Text book of Organic Chemistry-3<sup>rd</sup> Edn.-R.K. Bansal, (New Age, New Delhi) 1997.
14. Organic Chemistry-3<sup>rd</sup> Edn- F.A. Carey (Tata McGraw Hill, New Delhi) 1996.
15. K. Mislow: Introduction to Stereochemistry, Published by W.A.BENJAMIN, 1965, Bookbarn International (Bristol, SOM, United Kingdom).
16. Stereochemistry, Conformation and Mechanism-P.S.Kalsi (Wiley Eastern,New Delhi)1993.
17. Stereochemistry of Carbon Compounds- E. L. Eliel (Tata McGraw Hill, New. Delhi) 1994.

# ICH 403: PHYSICAL CHEMISTRY

## Course Objectives:

- To understand basic principle of quantum mechanics and thermodynamics.
- To learn reaction kinetics and its applications in understanding reaction mechanism.
- To study the causes, types and protection aspects of corrosion.
- To know metal finishing process, types and applications.
- To learn the application of electrochemistry in chloro alkali industries, electrosynthesis and electrochemical engineering.

## Unit I

14 hr

**Quantum mechanics:** Quantum theory and atomic spectra; the Bohr model, Photoelectric effect, de Broglie's hypothesis and wave-particle duality of material particles, Heisenberg's uncertainty principle, theory of wave motion, the wave function and its physical meaning, operators, Eigen values and Eigen functions, basic postulates of quantum mechanics, time independent Schrodinger wave equation, Application of Schrodinger wave equation to particle in a 1D box, 3D box, ring, harmonic oscillator and hydrogen atom. Tunneling, Approximate methods: Perturbation theory and variational methods. Introduction to molecular structure: Born Oppenheimer approximation, molecular orbital theory and valence bond theory.

## Unit II

14 hr

**Thermodynamics:** Terminology, Laws of thermodynamics. Heat changes in chemical reaction-Born-Haber cycle, bond energy, Kirchhoff's equation, flame and explosion temperature, calculation of heat of reaction. Free energy change and work function. Entropy-Evaluation, dependence on variables of a system, degradation of entropy. Entropy change in chemical reaction. Thermodynamics of mixing. Theory and determination of Chemical Potential. Liquid mixtures. Excess functions for non-ideal solutions.

**Chemical kinetics:** A brief review of basic concepts and terminologies in reaction kinetics. Rate law and factors effecting rate law. Steady state approximation. Complex reactions-reversible, parallel, consecutive and chain reactions, Explosive reaction ( $H_2-O_2$ )[qualitative aspects only].

## Unit III:

14 hr

**Corrosion:** Fundamentals of corrosion. Corrosion related damage, Types of corrosion (Galvanic, atmospheric, microbiological & stress). Methods of prevention & control (organic & inorganic coating, inhibitors, cathodic & anodic protection, material selection & design improvement). Corrosion problems in practice, passivity. Thermodynamics & kinetics of corrosion. Corrosion rate measurement (weight loss, Tafel extrapolation, polarization resistance) & monitoring. Concept & analysis of corrosion failure. Metal Finishing & Processing: Metal finishing & technological importance, Essentials of metal finishing, fundamentals of electrodeposition, effect of plating variables on the nature of electrodeposit, electroplating process, electroplating of copper, nickel, chromium & gold. Principles & applications of electroless plating, electrochemical etching, electrophoretic painting & electroforming.

## Unit IV:

14 hr

**Chlor-alkali Industry:** General concepts of brine electrolysis, modern technological developments, chlorine cell technologies, production of potassium hydroxide.

**Electrosynthesis:** Fundamentals of electro-organic & electro-inorganic synthesis, Kolbe's synthesis, electroreduction and oxidation of hydrocarbons, electroreduction of nitrocompounds, synthesis of adiponitrile. Electro-inorganic synthesis of fluorine, chlorate and ozone.

**Electrochemical Engineering:** Qualitative aspects of general considerations, costing of an electrolytic process, performance and figures of merit, electrolysis parameters, principles of cell design, laboratory data and scale up.

## Course outcome

The students would be learning the following topics

- The basic principle of quantum mechanics.
- The principles and applications of thermodynamics.
- Provides the general structure of thermodynamics.
- Basics and applications of chemical kinetics.
- The causes, types and protection aspects of corrosion phenomenon.
- Metal finishing process, types and applications.
- Application of electrochemistry in chloro alkali industries, electrosynthesis and electrochemical engineering.

## References:

1. Basic Quantum Chemistry, Harish Kumar Pandey.
2. Quantum Chemistry, Ira N. Levine, 5<sup>th</sup>edn., Prentice Hall of India Pvt. Ltd., 2006.
3. Quantum Chemistry, R. K. Prasad, 4<sup>th</sup> revised edition, New Age International (P) Ltd., New Delhi.
4. Quantum Chemistry, Donald A. McQuarrie, Viva Student Edition.
5. Principles of Quantum Chemistry, Ram Yatan Prasad & Pranitha, Cambridge University Press.
6. Thermodynamics for Chemists, S Glasstone, East-west Editon, New Delhi, 2003.
7. Chemical Thermodynamics-Basic Theory and Methods, 4<sup>th</sup>Edn., Klotz, Rosenbeg, Benjamin, 1986
8. Principles & Applications of Electrochemistry, D R Crow, 3<sup>rd</sup>Edn., Chapman & Hall,1987.
9. Chemical Kinetics, K J Laidler, Harper & Raw.
10. Chemical Kinetics-HareeshMehra, Alfa publishing, New Delhi, 2006
11. Industrial electrochemistry by and Walsh, F.C. II ed, Chapman and Hall (1990)
12. Modern Electrochemistry, Vol I, IIA & IIB(1998) J.O.M. Bockries and A.K.N.Reddy Springer
13. Engineering Chemistry by Jain and Jain 16 th ed, 2017.

## ICS 404: ENVIRONMENT, HEALTH AND SAFETY MEASURES

### Course objectives:

- To understand the environmental segments
- To study the various sources of pollutants, their adverse effect on living organisms and control.
- To study the various available water bodies and hydrologic cycle
- Understanding the maximum contamination level of pollutants in water bodies and their estimation techniques
- To learn the various aspects of quality of products
- To understand the safety and chemical and waste management

### UNIT I:

10 hr

**Air Pollution, Analysis & Control Methods:** Qualitative study of environmental segments, air pollutants, prevention & control, Green house gases & acid rain. Carbon monoxide, sources and control techniques. SO<sub>x</sub>-sources, control techniques-scrubbing, limestone injection process. Ozone hole & CFC's. Photochemical smog & PAN. NO<sub>x</sub> - Sources, NO<sub>x</sub> control techniques. Particulates: Size distribution, particulate collection-settling chambers, centrifugal separators, wet scrubbers, electrostatic precipitators & fabric filters. Analysis of air pollutants, Dispersion of air pollutants-weather, wind speed and acidity.

### UNIT II:

10 hr

**Water, Waste Water Treatment and Analysis:** Hydrologic cycle, sources, criteria & standards of water quality- safe drinking water, maximum contamination levels of inorganic & organic chemicals, radiological contaminants, and microbial contaminants. Public health significance & measurement of colour, turbidity, total solids, acidity, fluoride, alkalinity, hardness, chloride, residual chlorine, sulphate, fluoride, phosphate & different forms of nitrogen in natural & polluted water.

### UNIT III:

12hr

**Quality Control and Quality Assurance:** Role, Government standards like ISI, MINAS, Agmark, I.P., ASTM. Concepts of quality and quality control, the nature of variabilities. Specification and tolerances, sampling inspection, cost reduction and quality improvement experiments. Optimization.

Basic concepts of quality assurance, quality acceptance, sampling, reliability, cost aspects of quality decisions. Quality control in raw materials, production (in process) and finished product. Current trends in quality control, ISO 9000 and ISO 14000 series. Laws related to quality control. ISO 17025.

**Chemical Warfare Convention:** Definitions and schedules. Toxic chemicals, tear gas, chemical weapons, ocean dumping of chemical weapons.

### UNIT-IV:

10 hr

**Good Laboratory Practices:** Safety equipments, personal protective equipments, compressed gas safety, procedure for laboratory disposal of explosives, identification, verification and segregation of laboratory waste, disposal of chemicals in the sanitary sewer system, incineration and transportation of hazardous chemicals.

Emergency response-Chemical spills, radiation spills, biohazard spills, fires, medical emergency accident reporting, Safety rules of laboratory acquaintance of experimental set up and instruments,

Intellectual property and intellectual property rights. Data management, importance of safety and security of data. Experimental process and risk assessment

## Course Outcome

The student will be able to understand and apply

- Fundamentals, analysis and control methods of air and water pollution
- Quality control and quality assurance aspects used in industry and the laws regarding QA and QC along with chemical warfare convention.
- Thorough knowledge on good lab practices.

## References

1. Environmental Chemistry, A. K. Dey, 7<sup>th</sup> ed, New Age international Publishers, 2012.
2. Environmental Chemistry, S. K. Banerji, Prentice Hall India, 1993.
3. Environmental Chemistry, B. K. Sharma. 4th edition, GOEL Publishing House, New Delhi, 1998.
4. Chemistry of Water Treatment, S.D. Faust and O.M. Aly, Butterworths, 1983.
5. Environmental chemistry, Ahluwalia V. K., Anne Books India, 2008.
6. Chemistry for Environmental Engineering, Sawyer and McCarty, McGraw Hill, 1978.
7. Environmental Chemistry, I. Williams, John Wiley, 2001
8. Statistical Quality Control, 2<sup>nd</sup> Edn., Manohar Mahajan Dampat Rai and Sons, 1995.
9. Quality management: a process improvement approach, Fryman Mark A, Cengage learning, 2002.
10. Quality Control, Paranthaman D, Tata, McGraw Hill, 1987.
11. Gupta R. N. Chemical warfare and casualty management 2011
12. Vyas M. N. Safety and hazards management in chemical industries 2013. Atlantic publication.
13. Dikshith T. S. S Safety evaluation of environmental chemicals. New Age International, 1996.  
Chemical Safety Matters-IUPAC-IPCS, Cambridge Univ. Press, 1992

# ICS 405: PAPER AND TEXTILE TECHNOLOGY

## Course objectives:

1. To know fundamentals of Paper and textile technology.
2. To understand Pulp and paper science with pulp manufacturing.
3. To learn the techniques of Coating and recycling of paper and textile.

## UNIT I

12 hr

**Pulp and Paper Science:** Raw materials for paper, Important fiber producing plants, woody & non woody fibers used in paper industry, physical and chemical characteristics. Structure of wood, structural elements of wood and bark, cell wall & fiber morphology, chemical components of wood; **Pulp Manufacture:** Mechanical pulping, Thermomechanical and Refiner mechanical pulping, Semicheical & chemical pulping. Kraft pulping. **Papermaking:** Beating and Refining of pulp.

## UNIT II

10hr

**Textile Technology:** Brief history on origin of textiles. Introduction to textile fibers and basic requirements of textile fibers. Manufacture of eco-friendly regenerated fibre. Brief study of physical & chemical properties of cotton, wool, silk & bast fibers. Importance and need of ginning. Impurities in the cotton and remedies to minimize impurities in cotton.

## UNIT III

10 hr

Introduction to blending techniques and its types. Blends of Polyester/cotton and polyester/viscose. Introduction to synthetic fibres. Raw materials for productions of PET, modified viscose rayon and their applications. Brief out line on production of acetate and cupramonium rayon and their applications.

## UNIT IV

10 hr

**Coating and Recycling of paper and textile:** Introduction to coating of Paper and metal foils. Fillers used in papermaking. Pressing: Objectives, types of presses, Drying: Theory and types, Finishing: Unwinding and rewinding. Evaluation of Paper: Physical, optical, electrical properties and Chemical properties of paper. Objects of mixing and blending. Introduction to textile testing & quality control. Sampling techniques. Frictional, optical, electrical and thermal properties of textile. Recycling of paper and textile.

## Course Outcomes:

4. Fundamentals of Paper and textile technology.
5. Pulp and paper science with pulp manufacturing.
6. Coating and recycling of paper and textile.

## References

1. Bleaching of Pulp, R. P. Singh, TAPPI Press.
2. Joint Text Book Committee of the Paper Industry, Vol. I to X, Technical Editor Benjamin A. Thorp Series Editor Michael J. Kocurek, Published by the technical section Canadian Pulp and Paper Association.
3. Hand Book for Pulping and Papermaking, Christopher J. Biermann
4. Environmental Friendly Technologies for the Pulp and Paper Industries, Young and Akhtar TAPPI Press.
5. Hand Book for Pulp and Paper Technologists, Gary A. Smook
6. Formation of synthetic fibres, Walczalk.K. Gordon & Sci. London.
7. Manual of Cotton Spinning, Coulson. A.F.W. (Ed.), Vol. I to IV,
8. Textile Institute Pub., Manchester, 1989.
9. Spun Yarn Technology, Osteby, Butterworths, London, 1987.
10. Physical Testing of Textiles, B.P. Senville, Wood Head, 1999.
11. Principles of Textile Testing, Booth J. E., Butterworth, Wendon III Edition.
12. Technology of Textile Processing, Technology of Dyeing, Shenai, V.A. 4th Edn., Sewak Publications, Bombay, 1988

## ICP 406: INORGANIC CHEMISTRY PRACTICALS-I

### Objectives

- To establish broad knowledge of Inorganic Chemistry.
  - To impart the basic analytical and technical skills to work effectively in different fields of chemistry.
  - To perform accurate quantitative measurements with an understanding of the theory and use of contemporary chemical instrumentation, interpret experimental results, perform calculations on these results and draw reasonable, accurate conclusion.
  - To gain practical training in volumetric and gravimetric analysis and statistical analysis of data.
1. Analysis of Haematite-insoluble residue by gravimetry & Iron by volumetric method.
  2. Analysis of Dolomite-insoluble residue by gravimetry & Ca, Mg by complexometric method.
  3. Pyrolusite-Insoluble residue by gravimetry and Manganese content by oxalate method.
  4. Estimation of percentage of copper in brass.
  5. Determination of iron using potassium dichromate.
  6. Preparation of pure sample of ferrous ammonium sulphate (Mohr's salt)  $[\text{FeSO}_4 \cdot \text{NH}_4)_2\text{SO}_4 \cdot 6\text{H}_2\text{O}]$
  7. Preparation of pure sample of potash alum (Fitkari)  $[\text{K}_2\text{SO}_4 \cdot \text{Al}_2(\text{SO}_4)_3 \cdot 24\text{H}_2\text{O}]$
  8. Complexometric determination of Mn, Cu, Ni and Fe-Cr mixture
  9. Determination of Hardness of water.
  10. Analysis of Halide Mixture - Iodide by  $\text{KIO}_3$  and total halide by gravimetrically.
  11. Colorimetric Determination of Iron by thiocyanate and Cu by aqueous ammonia.
  12. Gravimetric Determinations of Mn, Ni, Mo, Pb/Cr, sulphide, thiocyanate.
  13. Spot test for the detection of inorganic ions (any ten cations).
  14. Statistical analysis of data.

### Course Outcome:

Students will have the ability to:

- Think critically and analyze chemical problems.
- Present scientific and technical information resulting from laboratory experimentation in both written and oral formats.
- Describe the principle, instrumentation and applications colorimetric analysis.
- Gravimetric determination of metal ions.
- Analysis of water samples.

### References

1. G.H. Jeffrey, J. Bassette, J. Mendham and R.C. Denny, Vogel's Text Book of Quantitative Chemical Analysis, 5<sup>th</sup> Edition, Longman, 1999.
2. Vogel, "Textbook of Qualitative Inorganic Analysis", 3 Edition, ELBS. 1976.
3. D.A. Skoog and D.M. West, Fundamentals of Analytical Chemistry, IV Edition, Old Reinhold & Winston, Publication, 1982.
4. B.K. Sharma, Instrumental methods of Chemical analysis, Goel Publishing House, 24th Edition, 2005.
5. Gurdeep R. Chatwal, Sham K. Anand, Instrumental Methods of Chemical Analysis, Himalaya Publication, 1979.

## ICP 407: ORGANIC CHEMISTRY PRACTICALS-I

### Course objectives

- To learn safety techniques while handling chemicals and glassware's.
- To get training on how to plan, execute single and multistep synthesis of organic small molecules.
- To purify and identify the products by physical and chromatographic methods.

**Single and Two stage organic preparations, purification and characterization:** Preparations of 1,2,3,4-tetrahydro carbazole, 7-hydroxy-4-methyl-coumarin, aspirin, adipic acid, Para red and Methyl red Preparations of p-bromo & p-nitroaniline from acetanilide, Ethyl resorcinol from Resorcinol,  $\epsilon$ -Caprolactam from cyclohexanone, p-Aminobenzoic acid from p-nitrotoludine, s-tribromo benzene from aniline, Benzylic acid from Benzoin, p- chlorotoluine from p-toludine, 2,4-Dinitrophenylhydrazine from Chlorobenzene, m- Nitrobenzoic acid from methyl benzoate, 2,4-Dinitrophenol from Chlorobenzene, o-Aminobenzoic acid from Phthalic anhydride, hydantoin from benzyl, p-amino azobenzene from Aniline, thiazoles from acetophenones, pyrimidines from aldehydes/ketones and thiourea, eosin from resorcinol & phthalic anhydride, Indigo from anthranilic acid, methyl orange from aniline, 5-hydroxy-1,3-benzothiole from hydroquinone, Benzimidazole from urea, Benzocaine from p-nitrotoluene, Dibenzyl from benzil, Benzil from benzoin, Benzalacetophenone dibromide from acetophenone.  
Any other interesting experiments.

### Course Outcome:

- Students gain the knowledge in single and two stage organic preparations, reaction monitoring using TLC, purification and its analytical characterisation.

### References:

1. Experimental Organic Chemistry–Vol. I & II–P. R. Singh et al, TMH New Delhi, 1981
2. Laboratory Manual in Organic Chemistry–Dey & Sitaraman, Allied , New Delhi, 1992.
3. Vogel's Text Book of Practical Organic Chemistry including Qualitative Organic Analysis- B. S. Furniss et al., Longman-ELBS, London, 1989.
4. Organic analytical chemistry, Theory and Practice-Jag Mohan, Narosa, 2003.
5. Practical organic chemistry by F.G. Mann & B.C. Saunders, 4<sup>th</sup> Edition, Longman, 1970.
6. Laboratory Manual of Organic Chemistry - Raj K Bansal, 2<sup>nd</sup> Edition, Wiley, 1990.
7. Systematic Lab Experiments in organic chemistry-Arun Sethi, New Age International, 2006.
8. Advanced Practical organic chemistry-Jag Mohan, Himalaya Publishing House, 1992.



# ICP 408: PHYSICAL CHEMISTRY PRACTICALS-I

## Course Objectives:

- To determine physical constants using refractometry, adsorption experiment and viscometry.
- To understand solution chemistry by the way of studying reaction kinetics and energetics.

## Any 12 experiments are to be carried out

1. Analysis of a binary mixture and determination of molar refraction of a solid and the composition of chloroform and acetone in its azeotropic mixture by refractometry.
2. Analysis of a binary mixture of two miscible liquids by viscometry and the relation between viscosity of a solution and the electrical conductivity.
3. Study of variation of viscosity of a liquid with temperature.
4. Determination of parachor value for CH<sub>2</sub> group by S.T method, the composition of a solution by S.T measurement and the CMC of a soap solution by S.T measurement.
5. Surface tension - concentration correlation for solutions (Gibbs equation).
6. Verification of Freundlich adsorption isotherms for acetic & oxalic acids on activated charcoal.
7. Analysis of a binary mixture by surface tension method.
8. Adsorption of iodine on charcoal from alcoholic solution.
9. Study of adsorption of picric acid on charcoal using a calorimeter.
10. Acid catalyzed hydrolysis of methyl acetate and determination of catalytic strength of an acid.
11. Saponification of ethyl acetate by conductivity method.
12. Reaction between potassium persulphate and potassium iodide (including the study of salt effect and catalysis by Ag<sup>+</sup>, Fe<sup>2+</sup> and Cu<sup>2+</sup> ions).
13. Decomposition of diacetone alcohol by NaOH & Hydrolysis of t-Butyl chloride.
14. Reaction between hydrogen peroxide and HI.
15. Determination of solubility of lead iodide at different Temperature and hence molar heat of solution.
16. Determination of heat of solution of a sparingly soluble solute.

## Course Outcome

Students will be able to

- Think critically and analyze chemical problems.
- Present scientific and technical information resulting from laboratory experimentation in both written and oral formats.
- Explain the physical constants using refractometry, adsorption experiment and viscometry.
- Account on hydrolysis, catalytic effect and calculation of thermodynamic parameters.

## References

1. B. P. Levitt, Longman, Findlay's Practical Physical Chemistry, J Wiley, London, 1954.
2. Experimental Physical Chemistry, Das & Behera, Tata McGraw Hill, New Delhi, 1983.
3. J.B. Yadav, 16<sup>th</sup> edition of Advanced Practical Physical Chemistry, Goel publishers, 1989.
4. Experiments in Physical Chemistry, J.C. Ghosh, Bharathi Bhavan, 1974.
5. D.A. Skoog and D.M. West, Fundamentals of Analytical Chemistry, IV Edition, Old Reinhold & Winston, Publication, 1982.
6. B.K. Sharma, Instrumental methods of Chemical analysis, Goel Publishing House, 24<sup>th</sup> Edition, 2005
7. Gurdeep R. Chatwal, Sham K. Anand, Instrumental Methods of Chemical Analysis, Himalaya Publication, 1979.

## II SEMESTER

### ICH 451: ANALYTICAL CHEMISTRY

#### Course Objectives:

- To understand different types of titrations and the errors.
- To learn different chromatographic techniques.
- To study different physical techniques.
- To learn the principle and applications of different spectroscopic and diffraction methods.

#### UNIT I

14

hr

Preparation of samples for analysis, nature of errors, statistical treatment of errors, the t- and F-tests, significant figures, rejection of data. Precipitation phenomena: Precipitation from homogeneous solutions, organic precipitants in inorganic analysis. Solvent extraction of metal ions, nature of extractant, distribution law, partition coefficients, types of extractions and applications. Theories of redox indicators, titration curves, feasibility of redox titrations. Chelometric titrations-titration curves with EDTA, feasibility of EDTA titrations, indicators for chelometric titrations, selective masking and demasking techniques, industrial applications of masking.

#### UNIT II

14 hr

Chromatographic Techniques: Principles, classifications and theory of chromatographic separations. Column chromatography: Principles, Differential migration, Separation of a mixture of o/p-nitroanilines

Gas Chromatography: Principles, columns, detectors-TCD, FID, ECD and column efficiency, capacity factors, resolution. Practical aspects of GC-Hypernated techniques. Liquid Chromatography HPLC: Principles, equipment, columns, detectors, choice of column, materials GC, GCMS and LCMS.

Ion exchange chromatography: Structures of resins, Types, Theory and apparatus, selectivity, Applications. Thin layer chromatography: Principles, selection of stationary and mobile phases, Preparative TLC, Applications Paper chromatography: Theory and principle. Techniques: one, two- dimensional and circular paper chromatography. Mechanism of separation, structure of cellulose and types of paper. Methodology- Factors affecting R<sub>f</sub> values. Advantages and applications.

#### UNIT III

14 hr

##### Electroanalytical Techniques

Introduction, theory, principle, methodology, instrumentation and application of the following techniques: Conductometry, Potentiometry, Coulometry, Voltammetry.

**Light -Scattering methods:** Nephelometry & turbidimetry theory, effects of concentration, particle size & wavelength on scattering, instrumentation & application.

**Fluorometry and phosphorimetry:** Introduction, fluorescence and phosphorescence, factors affecting fluorescence and phosphorescence, internal conversion, intersystem crossing (radiationless processes) quenching. theory, relationship between intensity of fluorescence and concentration, instrumentation- basic differences in the measurement of fluorescence and phosphorescence, spectrofluorometers, advantages and disadvantages

#### UNIT IV Advanced instrumental techniques:

14 hr

Spectrophotometry, Atomic spectroscopy

**Surface probe microscopy:** Atomic force microscopy, Scanning tunnelling microscopy, Field emission scanning electron microscopy, Transmission electron microscopy.

**Thermal Analysis-** TG, DTA and DSC- Principles and applications.

**X-ray diffraction techniques-** Powder and single crystal XRD, principle, techniques and applications.

**Course Outcome:**

- Students get to learn how to measure errors during estimations
- Chromatographic techniques namely, gas chromatography, liquid chromatography, ion exchange chromatography, TLC and paper chromatography.
- Electroanalytical techniques with advance instrumental technique such as surface probe microscopy, thermal analysis and X-ray diffraction analysis.

**References:**

1. Inorganic Chemistry, 3<sup>rd</sup> edn., G.L. Miessler and D.A. Tarr, Pearson Education inc.
2. Inorganic Chemistry, 4<sup>th</sup> edn., J.E Huheey, R.L.Keiter and A.L.Keiter, Addison Wesley,1993.
3. G.D. Christian, Analytical Chemistry, John Wiley, 1986.
4. Analytical chemistry-problems and solutions by S.M.Khopkar , New Delhi : New Age International (P) Ltd., 2002.
5. Analytical chemistry by G.L.David Krupadanam, D.Vijay Prasad, K.Varaprasad Rao, K.L.N Reddy, C. Sudhakar, Universities Press India Ltd,2002.
6. R.A. Day and A.L. Underwood: Quantitative Analysis, (Prentice Hall, India), 1998.
7. H.H. Wlliard, L.L. Merrit and J.J. Dean, Instrumental methods of analysis, 1988.
8. B.K. Sharma, Instrumental methods of chemical analysis, Goel publishing House, 2000.
9. Skoog, Holler and Nieman: Principles of Instrumental Analysis, Harcourt Acta, 2001.
10. Brown D R, Chromatogarphy, Ivy Publishing House,2001.
11. B.K. Sharma, Chromatogarphy, Krishna Prakashan media, 1997.
12. Bier, Milan E D, Electrophoresis: Theory methods and applications, Academic 1967.
13. A K Tareen and Kutty, Crystallpgraphy, University Press, 2002.
14. F.C. Ladd Mark & Palmer, R.A.: Structure Determination by X-ray Crystallography, 2003.
15. S. K. Chatterjee , X-Ray Diffraction theory and application, ISTE, 2007.
16. S. M Cannon, Comprehensive Inorganic Chemistry, , Newyork, 1972.
17. J.H. Kennady, Analytical Chemistry: Principles , Cengage Learning India Pvt.Ltd.
18. Dhanaraj, G., Byrappa, K., Prasad, V., Dudley, M. (Editors): Springer Handbook of Crystal Growth. © 2010.
19. A.G. Jackson: Handbook of Crystallography For Electron Microscopists and Others

# ICH 452: ADVANCED ORGANIC CHEMISTRY

## Course Objectives:

- To learn the role of organic reagents in organic synthesis and its applications in understanding reaction mechanism.
- To study the classification of natural products, its isolation and biological importance.
- To learn various named reactions and its applications in organic synthesis.
- To learn the chemistry of Carbohydrates.

## UNIT I

14 hr

### Reagents in Organic Synthesis

Uses of 1,3-dithiane, organoboranes, Trimethyl silyl iodide, Tri-n-butyl tin hydride, Selenium dioxide, Osmium tetroxide, Perbenzoic acid, Lead tetra acetate, Lithium aluminium hydride, Sodium borohydride, Organolithium, organomagnesium and Organo zinc compounds in organic synthesis and functional group transformations.. Synthetic applications of PTC, LDA, MnO<sub>2</sub>, Diazomethane, DCC, Gilman's reagent, DMAP.

## UNIT II

14 hr

### Organic Name Reactions and Rearrangements

Reactions, mechanisms and synthetic uses of Mannich reaction, Barbier-Wieland degradation, Oppenauer oxidation, Birch reduction, Claisen-Schmidt condensation, Cope and Hoffmann elimination, Vilsmeier-Haack reaction, Suzuki coupling, Woodward-Prevost hydroxylation, Swern oxidation Ugi, Biginelli and Mitsunobu reaction. Classification and general mechanistic treatment of nucleophilic, electrophilic & free radical rearrangements, Intermolecular & intramolecular migration, nature of migration & migratory aptitudes, Mechanisms of Wagner-Meerwein, Fries, Favorskii, Beckmann, Claisen, Neber & Smiles rearrangement.

## UNIT III

14 hr

### Natural product chemistry

Introduction to primary and secondary metabolites in plants. Extraction methods of chemical constituents from plants, such as fractionation using solvents, specific extraction of alkaloids and supercritical fluid extraction. Characterizations of isolated compounds (terpenes, sterols, alkaloids, carbohydrates, flavonoids and poly phenols) by colour reactions and spray reagents.

Structure elucidation of ocimene monoterpene, classification of pigments, structure elucidation of  $\beta$ -carotene. Biosynthesis of terpenes from mevalonic acid and sterols from squalene. Synthesis of quercetin. Structural elucidation of testosterone, androsterone, estrone and progesterone. Determination of carbon skeleton of alkaloids (Hofmann, Emde and Von Braun degradation methods). Structural elucidation of ephedrine, nicotine, atropine, hygrine.

## UNIT IV 14 hr

### Carbohydrates

Introduction, Ring size determination of Monosaccharides, conformational and configuration representations of monosaccharides, Mechanism of mutarotation, Base catalysed isomerization of aldoses and ketoses, Epimerization, Anomeric effect, Glycosides, ether and ester derivative of carbohydrate, Deoxysugars, oxidation and reduction reaction of carbohydrate. Disaccharides: Lactose, Maltose, and sucrose. Polysaccharides: Structure and degradation of starch, cellulose and glycogen. Industrial importance and biological importance of cellulose, starch, glycogen, dextran, hemicellulose, pectin, agar agar.

## Course Outcome

### The students will be learning the following

- Use of different reagents in organic synthesis and their industrial applications.
- Organic named reactions and rearrangements.
- Natural product chemistry with isolation, characterization and synthesis.
- The chemistry of Carbohydrates and their industrial importance.

### References:

1. Organic Chemistry, Vol-II, I. L. Finar. 3rd.ed., Longmans Green & Co. 1964.
2. Schaum's outline of theory and problems of Organic Chemistry, Harbert Meislich, Howard Nechamkin and Jacob Sharefkin. 2<sup>nd</sup> ed., Tata McGraw-Hill NewDelhi 2003.
3. Natural products: Their chemistry and biological significance, J. Mann, R. S. Davidson, J. B. Banthorpe and J. B. Harborne. Longman Scientific & Technical, 1994.
4. A text book of synthetic drugs, O. D. Tyagi and M. Yadav Modern Concepts of Advanced Organic Chemistry-R.P. Narein (Vikas, Delhi) 1997.
5. Name Reactions and Reagents in Organic Synthesis, Second Edition Bradford P. Mundy, Michael G. Ellerd, Frank G. Favaloro Jr., First ed, John Wiley & Sons, 2005.
6. Transition Metal Reagents and Catalysts: Innovations in Organic Synthesis, Jiro Tsuji, Wiley-Blackwell; Revised ed. Edition, 2002.
7. Carbohydrate Chemistry and applications of carbohydrates, K. M. Lokanatha Rai.
8. Carbohydrate Chemistry: Volume 40, Editors: Amelia Pilar Rauter, Thisbe Lindhorst, Yves Queneau RSC Publishing, 2014
9. A Text book of Organic Chemistry-Tewari, Vishnoi and Mehrotra (Vikas, NewDelhi) 1998.
10. A Text book of Organic Chemistry-3<sup>rd</sup> Edn.-R.K. Bansal, (New Age, New Delhi) 1997.
11. Organic Chemistry-3<sup>rd</sup> Edn- F.A. Carey (Tata McGraw Hill, New Delhi) 1996.

## Course Objectives:

- To study both conventional and nonconventional energy systems
- To learn Principle and application of colloidal chemistry in electrophoresis.
- To understand Adsorption phenomenon and its application.
- To know Petroleum and petrochemicals

## UNIT I:

14 hr

### Energy Systems

Chemical energy sources and their limitations (natural gas, coal, nuclear fusion, nuclear fission and Hydro power). Electrochemical energy systems-Introduction, classification, battery characteristics. Primary batteries-Laclanche dry cell (Zn and Mg), Alkaline MnO<sub>2</sub> batteries. Secondary batteries-Introduction, lead acid battery, Alkaline storage battery. Lithium batteries-The primary & secondary lithium batteries. Lithium based conducting polymer battery. Fuel cells-Introduction, efficiency, classification and types (H<sub>2</sub>-O<sub>2</sub> fuel cell, methanol fuel cell, solid polymer electrolyte fuel cell biofuel cell ).

## UNIT II:

14 hr

**Non conventional energy systems:**Solar energy cells-Introduction, semiconductor electrodes, semiconductor-electrolyte interface, parameter controlling efficiency, stability of semiconductor electrodes, Photoelectrochemical and photogalvanic cells. Production of Hydrogen, hydrogen energy. Applications of photochemistry-photoelectrocatalysis, photoreduction of CO<sub>2</sub> and photoelectrochemical waste removal. Hydrogen storage by metal and metal-alloys.

Wind energy-Atmospheric circulations, factors influencing wind and Betz limit. Formation of biomass, photosynthesis; Biomass resources. Chemical constituents and physicochemical characteristics of biomass; Biomass conversion processes; Biofuel, Petrocrops.

Ocean energy resources, Principles of ocean thermal energy conversion systems. Geothermal energy: Origin, types of geothermal energy sites.

## UNIT III:

14 hr

**Colloidal chemistry:** Introduction, Method of determining particle size. Donnan membrane, equilibrium and potentials, Importance and applications of colloidal chemistry. Theory, properties and applications of gels and emulsion. Migration of an ion in an electric field, factors affecting electrophoretic mobility. Types of electrophoresis-free electrophoresis, zone electrophoresis-paper and cellulose acetate electrophoresis, gel electrophoresis.

**Adsorption:** Introduction, types, Adsorption isotherms-Langmuir and BET(no derivation), Gibbs adsorption isotherm, applications of adsorption- surface area determination. Kinetics of gaseous reaction on solid surface-uni and bimolecular surface reactions (qualitative study), Catalysis: Types and industrial applications.

## UNIT IV:

14 hr

**Petroleum and Petrochemicals:** History of Petroleum-Origin, recovery and transportation, Composition of crude oils-Paraffins, Naphthenes, Aromatics, Sulphur compounds, Nitrogen compounds, Metallic constituents, Distillation-Pretreatment, atmospheric distillation, Vacuum distillation, Cracking-Thermal cracking, visbreaking, coking, catalytic cracking, hydrocracking, Reforming-Catalytic reforming.

**Hydrotreatment and Sulphur Recovery:** Finishing processes-Caustic washing, Merox process,

Hydrofining, methods for improving storage stability, filter, Molecular sieves Petroleum Products- LPG, LNG, Motor gasoline or Petrol, Diesel, Kerosene, Naphtha, Aviation turbine fuel, Heavy fuel oil, Bitumen, Lubricating oil, Greases, Petroleum waxes, Petroleum fractions for petrochemicals. Naphtha and Para xylene. General properties of petroleum products, alternative fuels.

### **Course Outcomes:**

- Students learn about types of renewable and non renewable sources of energy.
- Electrochemical energy systems pertaining to classical and modern batteries and also fuel cells
- Application of photoelectrochemistry and photoelectytic catalysis in waste removal and solar cell applications.
- Principle and application of colloidal chemistry in electrophoresis.
- Adsorption phenomenon and its application.
- Petroleum and petrochemicals: history, composition and reformation with finishing process namely hydro treatment.

### **References**

1. Engineering chemistry, Gadag R V, I K international, 2010.
2. Chemical and Electrochemical Energy Systems, Narayan R & B Viswanathan, University Press, 1998.
3. Energy Storage for Power Systems, Ter-Gazarian A., Peter Peregrinus, London, 1994.
4. Modern Electrochemistry, Vol 2A and B, JOM Bockris & AKN Reddy, Springer, NY, 1998.
5. Biochemical & Photosynthetic Aspects of Energy Production, Anthony San Pietro, Academic Press, N Y, 1980.
6. Bio Energy for Rural Energisation, R.C. Maheswari, Concepts Publication, 1997.
7. Wind Energy Systems, G L Johnson, Prentice Hall Inc, New Jersey, 1985.
8. Modern Petroleum Refining Process, 2<sup>nd</sup> Edn., Rao, IBH.
9. Introduction to Petrochemicals, Maiti, IBH.
10. A Text Book of Engineering Chemistry, M M Uppal, Khanna Publishers, 1986.
11. Modern Petroleum Chemistry-An overview, Kochu Baby, Manjaram & Kannatheri Publication, Kochi.
12. Colloids Chemistry, A.K.Sharma, Goel publishing House, Meerut, 1991.
13. Sequeira, A. Jr. Petroleum Processing Handbook. J.J. McKetta (Editor). Marcel Dekker Inc., New York. p. 634. 1992.
14. Walmsley, A.G. In Modern Petroleum Technology. G.D. Hobson and W. Pohl (Editors). Applied Science Publishers Inc., Barking, Essex, England. Chapter 17. 1973.

# ICS 454: CHEMICAL ENGINEERING TECHNOLOGY

## Course Objectives:

- To provide the detailed structure of unit operation and unit processes.
- To learn the basic design and concepts of operating instruments used in industries.
- To know the recent trends of unit operation involving flow chemistry.
- To distinguish the different reactions used in industrial processes.

## Unit Operations

### UNIT I:

10 hr

**Evaporation:** Types of evaporators, jacketed, horizontal and vertical tube evaporators, forced circulation evaporations, multiple effect evaporators.

**Distillation:** Boiling and distillation, vapor-liquid equilibria, Raoult's law & Henry's law, relative volatility, azeotropic mixtures, flash distillation, steam distillation, vacuum distillation, fractional distillation.

### UNIT II:

12 hr

**Crystallization:** Theory & mechanisms of growth of crystal, nucleation, saturation (Mier's theory), super saturation, types of crystallization, classification of crystallizers (agitated tank, Swenson Walkers, Krystal, Oslo, continuous vacuum crystallizers), caking of crystals, effect of impurities.

**Gas absorption:** Definition, examples, solution criteria for gas absorption, Characteristics, types, merits and demerits of plate and tower packing. Comparison of absorption and distillation,

**Flow chemistry: concepts and applications.**

### UNIT III:

10 hr

#### Unit Processes

Unit process and flow sheet. **Nitration:** Nitrating agents, kinetics and mechanism of nitration of aromatic compounds, nitration of paraffinic hydrocarbons, nitrate esters, N-nitrocompounds, typical industrial manufacturing process. **Sulfonation:** Sulfonating agents, kinetics and mechanism, desulfonation, work-up procedures. Industrial equipment and technique, Batch and continuous processes, manufacturing processes for detergents, dye intermediates, turkey red oil.

**Alkylation and acylation:** Alkylation & acylation at Carbon, Oxygen and Nitrogen, Friedel-Craft reaction, applications of active methylene compounds like diethyl malonate and ethyl acetoacetate. Industrial processes

### UNIT IV:

10 hr

**Catalytic hydrogenation and hydrogenolysis:** Different types of catalysts, Industrial hydrogenation processes. **Halogenation:** Kinetics & mechanism of halogenation reaction, survey methods, catalytic chlorination, manufacturing processes for chlorobenzene, BHC, chlorinated methanes, vinyl chloride. **Oxidation:** Oxidising agents with typical applications of each, liquid phase oxidation with oxidising compounds. **Esterification:** Kinetics and mechanism, esterification of carboxylic acid derivatives, esters by addition to unsaturated systems, industrial esterification, ethyl acetate, methyl methacrylate, cellulose acetate and nitroglycerin.



**Course Outcomes:**

1. Students learn about unit operations pertaining to evaporation, distillation and crystallization.
2. Unit processes and flow sheet for manufacturing of chemicals through sulphonation, nitration, alkylation and acylation; catalytic hydrogenation, oxidation and esterification.

**References**

1. F A Henglein, Chemical Technology, Fieser English edition, Pergamon, 1969.
2. J M Coulson, Chemical Engineering, Vol. I, II & III, Pergamon, 1964.
3. R N Shreve, The Chemical Process Industries, McGraw Hill Professional, 1984.
4. W L Badger, J T Bandchero, Introduction to Chemical Engineering, McGraw Hill Professional, 1955.
5. A Hougen, K M Watson, R A Ragetz, Chemical Process Principles, Vol I & II, John Wiley and sons, 1959.
6. John J McKetta Jr, Unit operations handbooks, Volume 1, CRC Press, 1992.
7. Warren L. McCabe, Julian C. Smith, Peter Harriott, Unit operations of chemical engineering, McGraw Hill Professional, 1956.
8. P H Groggins, Unit Processes in Organic Synthesis, McGraw Hill Professional, 5<sup>th</sup> Edition, 1995.
9. Engineering chemistry, Gadag R V, I K international, 2010.
10. Comprehensive industrial chemistry, More Prakash G, Pragathi Prakashan, 2010.

## ICS 455: CHEMICAL ANALYSIS IN AGRO AND FOOD INDUSTRIES

### Course objectives:

- To study the analysis of fuel and soil.
- To learn different types of fertilisers
- To study different types of insecticides, herbicides, fungicides, repellents.
- To learn the adulterants of food and its purification.

### Unit I

10 Hr

**Analysis of soil:** Moisture, pH, total nitrogen, phosphorous, silica, lime, Magnesia, Manganese, sulfur and alkali salts.

**Fuel analysis:** Solid, liquid and Gas, ultimate and proximate analysis heating values, grading of coal, liquid fuels, flash points, aniline point, octane number and carbon residue, gaseous fuels – producer gas and water gas – calorific value.

### Unit II

12 Hr

**Fertilisers:** Introduction, Essential plant Nutrients, Classification of Essential Nutrients, Primary Nutrients, Secondary Nutrients, Micronutrients, Macronutrients, Classification of Fertilizers- Straight Fertilizers, Compound/Complex Fertilizers, Fertilizer Mixtures, Feed Stock/ Raw materials- Nitrogenous Fertilizers, Phosphatic Fertilizers, Potassic Fertilizers, Manufacture and general properties of Fertilizer products- Intermediates- Ammonia, Nitric Acid, Sulphuric Acid, Phosphoric Acid, Nitrogenous Fertilizers- Ammonium Sulphate, Ammonium Nitrate, Calcium Ammonium Nitrate, Calcium Nitrate, Ammonium Chloride, Urea, Phosphatic Fertilizers, Ground Rock Phosphate, Single Superphosphate, Triple Superphosphate, Potassic Fertilizers- Potassium Chloride (Muriate of Potash), Potassium Sulphate (Sulphate of Potash), Potassium Nitrate, Complex Fertilizers- Ammonium Phosphate Sulphate, Ammonium Phosphates, Mono Ammonium Phosphate (MAP), Di-Ammonium Phosphate (DAP), Nitrophosphates, Urea Ammonium Phosphates, NPK Complex Fertilizers

### Unit III

10 Hr

**Insecticides:** Introduction, classification, Organochlorine insecticides-BHC, DDT, endosulfan, sevin, Insect pheromones, general introduction and applications in integrated pest management.

**Repellents:** Survey & synthesis of the repellents-N,N-diethyltoluamide, 2-ethyl-1,3-hexanediol.

**Fungicides:** Introduction, Inorganic & organic fungicides, Systemic fungicides-types & examples.

**Herbicides:** Introduction, study of sulfonyl ureas, Mechanism of action and toxicities of insecticides, fungicides and herbicides.

### Unit IV

10 Hr

**Food analysis:** Moisture, ash, crude protein, fat, crude fiber, carbohydrate, calcium, potassium, sodium, and phosphates, food adulteration – common adulteration in food, contamination of food stuffs, microscopic examination of foods for adulterants, Pesticide analysis in food products-Extraction and purification of sample, thin layer chromatography detection for organo phosphorous insecticide residues, thin layer chromatography for identification of Organo-chlorine pesticides in food products

**Course Outcomes:**

Students gain knowledge about the analysis of soil and food, determination calorific values of fuels, food analysis and clinical chemistry.

Students learn about different types of fertilizers, insecticides, fungicides, herbicides.

**Reference Books**

- 1) Food contaminants-Origin,propagation and analysis by S.N.Mahindru,2004
- 2) Food chemistry by Alex V Ramani, Tamil Nadu,2009
- 3) Methods on Physico-chemical analysis of fruits by Dr.B.C.Mazumdar and Dr.K.Mazumder,2003
- 4) A textbook of Fertilizers by Ranjan Kumar Basak,2007
- 5) Chemistry of Herbicides by Sree Ramulu, U S,1982
- 6) A laboratory manual for Environmental chemistry by R.Gopalan,Amirtha Anand,R.Wilfred Sugumar
- 7) Chemistry of insecticides and fungicides by Ramulu, U.S Sree.

**Course objectives**

- To learn instrumental techniques used in inorganic practical such as colorimetry, flame photometry
1. Colorimetric determination of Ti (IV) and Zr (IV)
  2. Simultaneous colorimetric determination of two metal ions – Mn and Cr.
  3. Flame photometric determination of Na, K, Li and Ca individually and in mixtures.
  4. Solvent extraction of Ni (II)
  5. Estimation of iron in cement by colorimetrically
  6. Determination of composition of complexes: a) Job's method: Fe-1, 10- Phenanthroline complex b) Mole ratio method: Zr-Alizarin red S complex, c) Slope ratio method: Cu ethylenediamine complex, d) Limiting logarithmic method: Uranyl sulphosalicylic acid complex.
  7. Determination of stability constants-Turner Anderson method: Fe-Tiron system,
  8. Cement analysis: i) SiO<sub>2</sub>-Gravimetrically ii) Calcium, Volumetrically iii) Iron, Volumetrically iv) Magnesium, Complexometrically iv) Aluminium, Gravimetrically.
  9. Determination of available chlorine in bleaching powder and residual chlorine in water samples.
  10. Determination of Iron present in sulpha- drugs; colorimetrically.
  11. Analysis of chalcopyrites, magnetite and ilmenite.
  12. Ion-exchange chromatography: Separation & determination of Mg<sup>2+</sup>/Zn<sup>2+</sup>, Zn<sup>2+</sup>/Cd<sup>2+</sup> & Cl<sup>-</sup>/Br<sup>-</sup>
  13. Determination of COD of a water sample and dissolved oxygen (DO) by Winkler's method
  14. Determination of nitrate & nitrite in water samples and seawater.
  15. Analysis of heavy metals in waste water, sea water (Pb, Hg etc. by spectrophotometry).
  16. Determination of available NPK in soil and fertilizer.
  17. Nephelometric determination of sulphate/phosphate.
  18. Determination of alkalinity of water samples.
  19. Determination of fluoride in drinking water by spectrophotometry and ion selective electrode.
  20. Determination of phosphates in detergents

**Course Outcome:**

- Instrumental techniques used in inorganic practical such as colorimetry, flame photometry and analysis of ore and minerals.

**References**

1. Vogel's Text Book of Quantitative Chemical Analysis (5<sup>th</sup> Ed), G.H. Jeffrey, J. Bassette, J. Mendham and R.C. Denny, Longman, 1999.
2. Sarvesh Kumar Dubey Asha Arora :A Practical Book on Soil Plant Water and Fertilizer Analysis, S.R. Scientific Publication. 2010.
3. Gupta PK, Soil, Plant, Water And Fertilizer Analysis (2nd Ed.), 2017.

## ICP 457: ESTIMATIONS AND EXTRACTIONS IN ORGANIC CHEMISTRY

### Course objective

- To study about the quantitative analysis of organic molecules by solution chemistry
- To learn extraction techniques of certain natural compounds.

Quantitative determination of sugars, amino acids, phenols, carboxylic acids, amides, esters, aldehydes, ketones, urea by various methods. Determinations of acid and ester; acid and amide in a mixture  
Determination of functional groups like hydroxyl, vic-hydroxyl, enol, amino, amide, unsaturation and nitro groups by various methods.

Extractions:

- Isolation of caffeine from Milk
- Isolation of caffeine from tea leaves
- Isolation of Piperine from black pepper
- Isolation of Nicotine from Tobacco
- Isolation of Hesperidin from Orange Peel Using Soxhlet Extractor

### Course Outcome:

- Quantitative determination of small molecules, biomolecules and functional groups.
- Students get laboratory training in extraction, characterization of natural products.

### References:

1. Elementary Practical Organic Chemistry, Vol. II, quantitative Organic Analysis-A.I.Vogel
2. Experimental Organic Chemistry, Vol. I &II, P.R.Singh, Tata McGraw-Hill,1981.
3. Practical Organic Chemistry- IV Ed- Dey &.Sitaraman, Allied, New Delhi,1992.
4. Laboratory Experiments in Organic Chemistry-Adam, Johnson &Wicon, McMillan,1979.
5. Experimental Organic Chemistry,.H.D.Durst&G.E.Goke, McGraw-Hill,1980
6. More Spectroscopic Problems in Organic Chemistry-A.J. Baker et al.,Heyden,1975.
7. Spectral Problems in Organic Chemistry,Davis& Wells, Chapman &Hall,1984.
8. Elementary Practical organic chemistry, Part 2: Quantitative organic analysis by Arthur I. Vogel, 2<sup>nd</sup> Edition, CBS Publishers and distributors,1987.
9. Organic analytical chemistry, Theory and Practice-Jag Mohan, Narosa,2003.
10. Laboratory Manual of Organic Chemistry - Raj K Bansal, 2<sup>nd</sup> Edition, Wiley,1990.
11. Systematic Lab Experiments in Organic Chemistry-Arun Sethi, New age International, 2006.

# ICP 458: ELECTROANALYTICAL TECHNIQUES

## Course Objectives:

- To establish broad knowledge of Physical Chemistry.
- To determine the concentration of analytes by electrochemical methods conductometry and potentiometry.

## Electrochemistry:

### A. Conductometry (At least 5 experiments to be carried out)

1. Determination of hydrolysis constants (aniline hydrochloride etc.).
2. Titration of a mixture of acetic acid, monochloro and trichloroacetic acids with NaOH.
3. Determination of concentrations/amounts of sulphuric acid, acetic acid and copper sulphate using sodium hydroxide.
4. Measurements of the conductance of a weak acid, HOAc and of the strong electrolytes NaOAc, HCl and NaCl and to calculate the ionization constant of the acid.
5. Analysis of the mixture of HCl and  $\text{NH}_4\text{Cl}$ .
6. Determination of activity coefficient of Zinc ions in 0.002 M  $\text{ZnSO}_4$ .
7. Determination of equivalent conductance's and dissociation constants of weak acids.

### B. Potentiometry (At least 7 experiments are to be carried out)

8. Determination of pK values of phosphoric acid by potentiometric titration with sodium hydroxide using glass electrode.
9. Determination of acidic & basic dissociation constants and isoelectric point of an amino acid.
10. Determination of the potential of an electrochemical cell and mean ionic activity coefficient.
11. Determination of activity coefficient of an electrolyte at different molalities.
12. Determination of pH of buffer solutions with a pH meter & evaluation of  $\text{pK}_a$  of acids
13. Determination of thermodynamics of a cell reaction
14. Determination of  $\text{pK}_a$  values of mono, di and tri-acid base.
15. Determination of solubility of insoluble silver halide and the standard electrode potential using quinhydrone electrode
16. Determination of degree of hydrolysis of  $\text{CH}_3\text{COONa}$  and  $\text{NH}_4\text{Cl}$ .
17. Determination of hydrolysis constant of aniline hydrochloride.
18. Verification of Nernst equation for  $\text{Ag}^+$ ,  $\text{Cu}^{2+}$  and  $\text{Zn}^{2+}$  species.
19. Determination of transport number of ions by emf method ( $\text{Ag}^+$ ,  $\text{Cd}^{2+}$ ,  $\text{NO}_3^-$ ,  $\text{SO}_4^{2-}$ )
20. pH titration of (a) HCl versus NaOH, (b)  $\text{CuSO}_4$  versus NaOH and (c) HOAc versus NaOH and (d) lead nitrate versus potassium chromate.
21. Potentiometric titration of halides in mixtures ( $\text{Cl}^-$ ,  $\text{Br}^-$  and  $\text{I}^-$ ) with silver nitrate.
22. Potentiometric determination of dissociation constants of weak acids.

### **Course Outcome:**

Students will be able to

- Think critically and analyze chemical problems.
- Present scientific and technical information resulting from laboratory experimentation in both written and oral formats.
- Accounts on potentiometric and conductometric titrations.

### **References**

8. B. P. Levitt, Longman, Findlay's Practical Physical Chemistry, J Wiley, London, 1954.
9. Experimental Physical Chemistry, Das & Behera, Tata McGraw Hill, New Delhi, 1983.
10. J.B. Yadav, 16<sup>th</sup> edition of Advanced Practical Physical Chemistry, Goel publishers, 1989.
11. Experiments in Physical Chemistry, J.C. Ghosh, Bharathi Bhavan, 1974.
12. D.A.Skoog and D.M.West, Fundamentals of Analytical Chemistry, IV Edition, Old Reinhord & Winston, Publication, 1982.
13. B.K. Sharma, Instrumental methods of Chemical analysis, Goel Publishing House, 24<sup>th</sup> Edition, 2005
14. Gurdeep R. Chatwal, Sham K. Anand, Instrumental Methods of Chemical Analysis, Himalaya Publication, 1979.

## ICE 459: INDUSTRIAL SAFETY, ENVIRONMENTAL AND ELECTROCHEMICAL SCIENCES

### Course objectives:

- To learn general safety aspects in industry, chemical warfare convention.
- To know about QA and QC, environment problems such as air and water pollution.
- To understand causes for Corrosion and protecting methods for it

### Unit:

10 hr

**Safety:** Flammable material handling and fire fighting equipments, control measures for toxic chemicals, industrial hygiene, safety in laboratories & plant, safety in the transportation & storage of chemicals. OHSAS 18000.

**Chemical Warfare Convention:** Definitions and schedules. Toxic chemicals, remote control systems, tear gas, chemical weapons, ocean dumping of chemical weapons.

### Unit II:

12 hr

**Quality Control and Assurance:** Role, Government standards like ISI, MINAS, Agmark, I.P ASTM. Concepts of quality and quality control, the nature of variabilities. Specification and tolerances, sampling inspection, cost reduction and quality improvement experiments. Optimization. Basic concepts of quality assurance, quality acceptance, sampling, reliability, cost aspects of quality decisions. Quality control in raw materials, production (in process) and finished product. Current trends in quality control, ISO 9000 and ISO 14000 series. Laws related to quality control. ISO 17025.

### Unit III:

10 hr

**Air Pollution:** Qualitative study of environmental segments, air pollutants, prevention & control, Green house gases & acid rain. Ozone hole & CFC's. Photochemical smog, PAN and Bhopal Gas tragedy.

**Water, Waste Water Treatment and Analysis:** Hydrologic cycle, sources, criteria & standards of water quality- safe drinking water. Public health significance & measurement of colour, turbidity, total solids, acidity, fluoride, alkalinity, hardness, chloride, residual chlorine, sulphate, fluoride and phosphate in natural & polluted water. Significance of DO, BOD & COD. Water purification for drinking & industrial purposes, disinfection techniques, demineralization, desalination processes & reverse osmosis.

**Energy systems:** Chemical energy sources and limitations. Electrochemical energy sources. Principle and importance of primary(dry cell), secondary (Lead-acid battery) and fuel cells ( H<sub>2</sub>-O<sub>2</sub>). Basics of solar energy system. Safety implications. Energy from wind, ocean, geothermal and biomass.

### Unit IV:

10hr

**Corrosion:** Fundamentals of corrosion. Corrosion related damage, Types of corrosion. Methods of prevention & control (organic & inorganic coating, inhibitors, cathodic & anodic protection, material selection & design improvement). Corrosion problems in practice, passivity.

**Metal Finishing & Processing:** Metal finishing & technological importance, fundamentals of electrodeposition, electroplating process (copper and Nickel). Principles & applications of electroless plating.



**Paints:** Classification of paints, types, Constituents of paints. Requirements of a good paint. Emulsion paints. Paint removers.

**Electrochemistry of Environment:** Global warming, role of electrochemistry in the transport system, fixing of CO<sub>2</sub>, sewage disposal and treatment of waste

### Course Outcomes:

- It is an open elective course student learns safety aspects in industry, chemical warfare convention.
- QA and QC, environment problems such as air and water pollution.
- Corrosion causes and inhibition

### References

1. Environmental Chemistry, A. K. Dey, 7<sup>th</sup> ed, New Age international Publishers, 2012.
2. Environmental Chemistry, S. K. Banerji, Prentice Hall India, 1993.
3. Environmental Chemistry, B. K. Sharma. 4th edition, GOEL Publishing House, New Delhi, 1998.
4. Chemistry of Water Treatment, S.D. Faust and O.M. Aly, Butterworths, 1983.
5. Environmental chemistry, Ahluwalia V. K., Anne Books India, 2008.
6. Chemistry for Environmental Engineering, Sawyer and McCarty, McGraw Hill, 1978.
7. Environmental Chemistry, I. Williams, John Wiley, 2001
8. Statistical Quality Control, 2<sup>nd</sup> Edn., Manohar Mahajan Dampat Rai and Sons, 1995.
9. Quality management: a process improvement approach, Fryman Mark A, Cengage learning, 2002.
10. Quality Control, Paranthaman D, Tata, McGraw Hill, 1987.
11. Gupta R. N. Chemical warfare and casualty management 2011
12. Vyas M. N. Safety and hazards management in chemical industries 2013. Atlantic publication.
13. Dikshith T. S. S Safety evaluation of environmental chemicals. New Age International, 1996.
14. Chemical Safety Matters-IUPAC-IPCS, Cambridge Univ. Press, 1992.
15. Engineering chemistry, Gadag R V, I K international, 2010.
16. Chemical and Electrochemical Energy Systems, Narayan R & B Viswanathan, University Press, 1998.

# III SEMESTER

## ICH 501: SPECTROSCOPIC TECHNIQUES

### Course Objectives:

1. To understand molecular spectroscopy techniques namely vibrational and Raman spectroscopy.
2. To learn the theory and application UV, IR, NMR and mass spectroscopy in structure determination of organic molecule.
3. To learn structure elucidation by solving composite spectral problems.

### UNIT I

14 hr

Introduction to spectroscopic techniques, intensity of spectral lines, natural line width and line broadening. Rotational, vibrational and electronic energy levels and selection rules. **Microwave Spectroscopy:** The rotation and classification of molecules, rotation spectra of diatomic and polyatomic molecules. Rigid and non-rigid rotator models. Determination of bond lengths, isotope effect on rotation spectra. Stark effect, nuclear and electron spin interaction. Microwave Spectrometer.

**Vibrational Spectroscopy:** Vibration spectra of diatomic molecules - linear harmonic oscillator, vibrational energies, zero point energy, force constants & bond strengths; anharmonicity of molecular vibrations- Morse PE diagram, selection rules, fundamental, overtones and hot bands. Vibrations of polyatomic molecules- normal modes of vibrations & nature of molecular vibrations (Ex-CO<sub>2</sub> & H<sub>2</sub>O). **Vibration-rotation spectra** of diatomic and polyatomic molecules, selection rules, PQR branches.

**Raman spectroscopy:** Introduction, theory and applications of Raman spectra, mutual exclusion principles and its applications.

### UNIT II

14 hr

**Application of infrared spectroscopy** in the structural study-identity by fingerprinting and identification of functional groups. Characteristic vibrational frequencies of common functional groups (alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols and amines). Study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides and acids). Factors affecting band positions and intensities-hydrogen bonding, phase and solvent.

**UV/Electronic Spectroscopy:** Basic principles, Beer-Lambert law, molar absorptivity, energy levels, types of electronic transitions. Franck - Condon principles, ground and excited electronic states of diatomic molecules. Chromophores, auxochromes, electronic spectra of polyatomic molecules. Emission spectra, spectra of transition metal complexes, charge transfer spectra. Instrumentation and application. Factors affecting the positions of UV bands. Electronic transitions and empirical correlations of predicting  $\lambda_{\max}$  of organic compounds. Woodward-Fieser rules. UV absorption of aromatic compounds - effect of substituents and solvent effects. Empirical rules to calculate  $\lambda_{\max}$ . Application of UV spectroscopy in the structural study of organic molecules.

### UNIT III

14 hr

**Nuclear Magnetic Resonance Spectroscopy:** Magnetic properties of nuclei, theory and measurement techniques, NMR spectrometer, solvents used, chemical shift and its measurements, factors affecting chemical shift. Integration of NMR signals, spin-spin coupling, coupling constant. Shielding and deshielding. Chemical shift assignment of major functional groups, Classification (AX, AMX, ABX), spin decoupling; effects of chemical exchange, fluxional molecules, Hindered rotation through NMR spectrum, Karplus relationships (Karplus curve), double resonance techniques, solvent effects and Nuclear Overhauser Effect.

**NMR of nuclei other than proton:**  $^{13}\text{C}$  chemical shift & factors affecting it, Coupling constants. Decoupling-Noise decoupling & broad band decoupling. Off-resonance proton decoupling-some representative examples. 2D NMR techniques.

#### **UNIT IV: 14 hr**

**Mass Spectrometry:** Basic principles, interpretation of mass spectra, molecular ions, meta- stable ions and isotope ions, ion abundance. Fragmentation processes-representation of fragmentation, basic fragmentation types and rules. McLafferty rearrangement. Fragmentations (fragmentation of organic compounds with respect to their structure determination) associated with functional groups- alkanes, alkenes, cycloalkanes, aromatic hydrocarbons, halides, alcohols, phenols, ethers, aldehydes, ketones, carboxylic acids, esters, amides, acid chlorides, nitrocompounds and amines, retro Diels-Alder fragmentation and Nitrogen rule.

**Composite problems** involving the applications of UV, IR,  $^1\text{H}$  and  $^{13}\text{C}$  NMR and mass spectroscopic techniques.

#### **Course Outcomes:**

The course will make a student well versed in

- Molecular spectroscopy technique namely vibrational and Raman spectroscopy.
- Applications of UV, IR, NMR and mass spectroscopy in structure determination of organic molecule.
- Application of spectroscopy by solving composite problems.

#### **References**

1. Organic spectroscopy, William Kemp, 3<sup>rd</sup> Edn., PALGRAVE, 1991.
2. Organic spectroscopy: Principles and applications, Jagmohan, 2<sup>nd</sup> Edn., Narosa, 2007.
3. I.L. Finar Organic Chemistry Vol I 6th edition ELBS Longman 1973
4. Fundamentals of Molecular Spectroscopy IV ed., C. N. Banwell & E. M. McCash Tata McGraw- Hill Publishing Company Ltd., 1994.
5. Organic Analytical Chemistry Theory and Practice, Jag Mohan, Narosa Publishing House 2003
6. Spectrophotometric Identification of Organic Compounds, R.M. Silverstein, F.X. Webster, 6th Ed., John Wiley & Sons, Inc, New York, 2004.

# ICH 502: INDUSTRIAL CATALYSIS AND GREEN CHEMISTRY

## Course objective:

- To study in detail about the types and applications of catalysts
- Understanding the role of organometallic compounds as catalysts
- To learn about nanocatalysts and their applications
- To understand green chemistry techniques.

## UNIT I:

14 hr

Preparation of catalyst and their behaviour, Selection, preparation and evaluation of catalysts-test reaction, promoters, carriers and stabilisers, Role of supports, preparation & structure of supports, silica, alumina, silica-alumina, zeolites, carbon catalyst manufacture, catalyst size and shape, pre-treatments, deactivation process, sintering, poisoning and catalyst fouling.

**Definition of performance criteria of catalysts:** Activity, selectivity, temperature response, catalyst life. Surface active agents, classification of surface active agents, micellisation, hydrophobic interactions, critical micellar concentration (CMC), factors affecting the CMC of surfactants.

## UNIT II:

14 hr

### Catalysis by Organometallic Compounds:

Transition metal hydrides: Synthetic routes, structure and reactivity, synthetic applications. (Pd, Ni, Fe, Co, Ti complex); Coordinative unsaturation, oxidative addition and reductive elimination and insertion reactions, olefin hydrogenation, Wilkinson's Catalyst, Wacker process, Zeigler-Natta process, olefin metathesis, Monsanto process for the synthesis of acetic acid, heterogenization of homogeneous catalysts using polymer supports.

## UNIT III:

14 hr

### Catalysis by Nanocatalysts

Synthesis of Nanoporous Catalysts Microporous materials: Zeolites- Zeotypes – Overall steps in zeolite crystallization- Zeolite synthesis via.- dry gel route- Zeolite Y- determination of surface acidity- shape-selectivity; Mesoporous aluminosilicates: Synthesis of Mesoporous Silica- MCM-41-SBA-15; Aluminophosphates; Mesoporous Carbon- Sulfated Zirconia- Ag/SiO<sub>2</sub> composite nanocatalysts. Nanophotocatalysis and Catalysis of Gold nanocrystals Introduction to photocatalysis: Principle- Band energy engineering- Degradation of dye, Hydrogen generation- Organic synthesis.

## UNIT III:

14 hr

### Green Chemistry

Definition and principles, planning a green synthesis in a chemical laboratory, Green preparation- Aqueous phase reactions, solid state (solventless) reactions, photochemical reactions, Phase transfer catalyst catalysed reactions, enzymatic transformations & reactions in ionic liquids. Synthesis using scavenger resins, catalysis and biocatalysis.

Sonochemistry: Introduction, instrumentation, the phenomenon of cavitation, types of sonochemical reaction, Sonochemical esterification, substitution, addition, oxidation, reduction and coupling reactions. Microwave induced organic synthesis: Introduction, reaction vessel and reaction medium, concept, specific effect, atom efficiency, % atom utilisation, advantages and limitations, alkylation of active methylene compounds, N-alkylation, condensation of active methylene compounds with aldehydes, Diels-Alder reaction, Leuckardt reductive amination of ketones, ortho ester Claisen rearrangement and synthesis of enaminketones.

## Course Outcome

The students will learn the following

- Preparation of catalyst and their applications in industry.
- Utility of organometallic compounds in catalysis.
- Synthesis and application nanocatalysts

## References

1. Heterogeneous Catalysis, D.K. Chakrabarty and B. Viswanathan, New Age International (P) Limited, 2008
2. Nanoporous Materials: Synthesis and Applications, Edited by Qiang Xu, CRC Press, 2013
3. Catalysis: Principles and Applications, Edited by B. Viswanathan, S. Sivasanker, A.V. Ramaswamy, Narosa Publishing House, 2011
4. Photocatalysis, Edited by Masao Kaneko, Ichiro Okura, Springer, 2003.
5. New and Future Developments in Catalysis, Edited by Steven L. Suib, Elsevier, 2013.
6. Catalysis by Gold, Geoffrey C. Bond, Catherine Louis, David T. Thompson, Imperial College Press, 2006.
7. Green Chemistry edited by Bela Torok Timothy Dransfield , Elsevieer,2017.
8. New Trends in Green Chemistry, V.K.Ahluvalia ,1<sup>st</sup> ed, Springer Nature, 2019.
9. Green Chemistry, Theory and Practice, Paul T. Anastas and John C. Warner, Oxford University Press, 1998, New York, USA.
10. Real-World Cases in Green Chemistry, Michael C. Cann, Mare E. Connelly, American Chemical Society, 2000.
11. Green Chemical Synthesis and Processes, Paul T. Anastas, Luren G. Heine and Tracy C. Williamson (Editors), ACS Publication 2000.
12. Green Chemistry in India, M. Kidwai, Pure and Applied Chmistry, Vol. 73, No.8, 1261-1263,2001.
13. Pure and Applied Chemistry, Special Topic Issued on Green Chemistry, IUPAC, Vol. 72, No.7, July 2000.
14. Organic Synthesis: Speical Techniques, V. K. Ahluwalia and Renu Aggarwal, Narosa Publishing House, 2001, New Delhi.
15. Green Chemistry: An Introductory Text, Mike Lancaster, Green Chemistry Network, University of York, RSC, 2002.
16. Green Chemistry in Indian Context: Challenges Mandates and Chances of Success, Upasana Bora, Mihir K. Chaudhri and Sanjay K. Dehury, Current Science, Vol. 82,1427,2002.
17. Organic Synthesis in Water, Paul A. Grieco (Editor), Blackie Academic and Professional, London, UK.
18. Organic Reactions in Aqueous Media, CHAU-JUN Li and TAK-Hang Chan, John Wiley & Sons Inc., New York.

# ICH 503: SYNTHETIC, HETEROCYCLIC AND MEDICINAL CHEMISTRY

## Course Objectives:

- To study the retrosynthetic analysis for planning a synthesis, especially of complex organic molecules.
- To give a knowledge about pericyclic reactions.
- To learn synthesis, reactivity and industrial applications of heterocyclic compounds.
- To know about drugs, its synthesis and mode of action,

## UNIT I: Planning and Execution of Multistep Synthesis

14 Hr

Basic principles and technologies used in disconnection approach, synthons and synthetic equivalents, Interconversion of functional groups, one group C-X and two group C-X disconnections. Protecting groups-Principles of protection of hydroxyl, amino, carboxylic and carbonyl groups. Use of C-C one group and C-C two group disconnections in the synthesis of 1,2; 1,3; 1,4; 1,5 and 1,6-difunctionalised compounds. Retrosynthetic analysis of alcohols, carbonyl compounds, cyclic and acyclic alkanes, benzocaine, p-methoxyacetophenone, acetocyanohydrin, 2-methyl-6-methoxy-indole-3-acetic acid, 6-methylquinoline and. Illustrative synthesis of Juvabione, Longifolene, Prelog-Djerassi lactone, Solid phase synthesis of polypeptides.

## UNIT-II: Pericyclic chemistry

14 Hr

**Pericyclic Reactions:** Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl systems. Classifications of Pericyclic reactions. Woodward-Hoffmann correlation diagram and FMO approach.

**Electrocyclic Reactions:** Introduction, Con-rotatory and dis-rotatory Process,  $4n$  and  $4n+2$  systems. Reactions of cations and anions.

**Cycloaddition reaction:** Suprafacial and Antarafacial addition,  $2+2$  and  $4+2$  systems, 1,3-dipolar cycloaddition reactions and their applications in the synthesis of five membered heterocycles.

**Sigmatropic reactions:** Suprafacial and Antarafacial shift of H, [1,3] and [3,3]-sigmatropic shifts. Claisen, Cope, Oxy-Cope and Aza-Cope rearrangements.

## UNIT III: Heterocyclic Compounds

14 Hr

Hantzsch-Widman system for naming monocyclic, fused and bridged heterocycles. Chemistry of derivatives of pyrazole, imidazole, oxazole, thiazole, benzofuran, indole, benzothiophene, pyridine, quinoline. Inter conversion of coumarin to benzofuran, pyrrole to pyridine, Pyrimidine to pyrazole, indole/isatin to quinoline, furans to pyrrole. Uses of furan, pyrrole, thiophene in the synthesis of non-heterocycles.

## UNIT IV: Medicinal chemistry

14 Hr

Concept of lead compounds, analogues and prodrug, Factors governing drug design ADME, drug design through molecular disjunction and conjunction. Drug receptor interactions- Forces involved in drug receptor interactions Theories of drug action-occupancy, rate, induced fit theory. Concept of fragment based drug discovery. Structurally specific and non-specific drugs, Classification, synthesis and mode of action of following classes of drugs-Antipyretic analgesics (Cinchophen), General anaesthetics (Thiopental sodium), Local anaesthetics (benzocaine), cardiovascular drugs (diazoxide), antimalarials (chloroquine phosphate), antineoplastic agents (methotrexate and fluorouracil), antiviral drugs (methisazone).

## Course Outcomes:

### The students will be learning the following

- Planning and execution of multistep synthesis with retro synthetic approach.
- Different types of pericyclic reactions and its advantages.
- Reactivity, preparations and applications of heterocyclic compounds.
- Classification, synthesis and mode of actions of some drugs.

### References

1. Organic Synthesis-Special Techniques, V.K.Ahluwalia and R. Aggarwal, Narosa, New Delhi, 2001.
2. Organic Synthesis, R.E.Ireland, Prentice Hall India,1969.
3. Advanced Organic Chemistry, IV Edn., Part A &B, F.J.Carrey&R.J.Sundberg, Kluwer, 2001.
4. Organic Synthesis- A Disconnection Approach,Stuart
5. Art in Organic Synthesis, Anand, Bindra&Ranganath, Wiley, New Delhi,1970.
6. Modern Methods of Organic Synthesis, N. Carruthers, Cambridge University,1996.
7. Organic Reaction Mechanisms, V.K.Ahluwalia&R.K.Parashar, Narosa,2006
8. Heterocyclic Chemistry, J. Joule & G. Smith, Van-Nostrand, ELBS,1978.
9. Comprehensive Heterocyclic Chemistry, Vol.I-VI Edn., Katritzky& Rees, Pergamon,1984.
10. Heterocyclic Chemistry, Raj K. Bansal, New Age International,1999.
11. Medicinal Chemistry, Ashuthosh Kar, Fourth edition, New Age International PvtLtd.
12. Pericyclic reactions, S. M. Mukherji (The McMillan Bangalore),1979.
13. V.K. Ahluwalia and Mahu Chopra, Medicinalchemistry.
14. Graham L Patrick, An introduction to medicinal chemistry,Oxford.
15. Ashutosh Kar, Medicinal chemistry.
16. Frank Jensen, Introduction to Computational Chemistry, Wiley Publisher, Second Edition,2006.
17. Johann Gasteiger (Editor), Thomas Engel (Editor), Chemoinformatics: A Textbook, Wiley Publisher ISBN: 978-3-527-30681-7, 2003.
18. Rajarshi Guha (Editor), Andreas Bender (Editor), Computational Approaches in Cheminformatics and Bioinformatics Wiley-Blackwell, 2012.
19. Fan Li, Developing Chemical Information Systems: An Object-Oriented Approach Using enterprise JAVA, John Wiley & Sons, 2006,ISBN,0470068787, 978047006878

## ICS 504: Polymers and Soft materials

### Course Objectives

- To learn polymer chemistry and properties and synthetic methods.
- To know the versatility of polymer materials in their applications
- To provide the knowledge of basic concepts of liquid crystals and its applications.
- To learn the aspects of soft materials and organic solids with structural details.

### UNIT I

10 hr

#### Polymers

Basic concepts and techniques in polymer chemistry. General structures & classifications of polymers. Techniques of polymerization and molecular weight determination. Uses of some commercial and engineering polymers. Thermoplastics, thermosets and elastomers. Polymer processing techniques, additives for improvement of polymer properties, spinning of industrial polymers, wet, dry melt spinning and electrospinning.

**UNIT II****12 hr**

Polymer blend and composites -preparation and uses. Introduction to nano composites. Polymers as separation devices-principles and applications of reverse osmosis, ultra and nano filtration and electro dialysis, Uses in food industry and biotechnology. Medical applications of polymers: Concepts and design of oral, transdermal and targeted drug delivery systems-micro, macro and nano sized systems. Biodegradable polymers- Sources of plastic waste, waste management techniques.

**UNIT III****10 hr**

**Liquid Crystals:** Definition, Liquid crystal phases, Thermotropic liquid crystals, Nematic phase, Smectic phases, Chiral phases, Cholesterics, Lyotropic liquid crystals –Hexagonal columnar phase, Micellar cubic phase, Liquid crystalline phases, Theoretical treatment of liquid crystals-Parameter to describe a liquid crystals, optical properties of liquid crystals, LCD.

**Organic NLO and LED materials:** Introduction, phenomena, fabrication and applications.

**UNIT II:****10 hr**

**Soft Materials:** Thin Films and Langmuir-Blodgett Films, Preparation techniques, vaporation/sputtering, chemical process, MOCVD, sol-gel etc. growth technique, photolithography, properties and applications of thin and L-B films.

**Organic Solids and Fullerenes:** Conducting organics, organic superconductors, magnetism in organic materials. Fullerenes: doped fullerenes as superconductors.

**UNIT III:****10 hr****Course Outcome**

- Student will be understanding the versatility of polymers their uses in diverse fields and also understands the chemistry of polymers
- Students learn about fundamental of liquid crystal and their application in LCD technology.
- Also learn about Thin films processes and applications.

**References**

1. Material science and Engineering, W D Callister, Wiley 7<sup>th</sup> ed., 2007.
2. Liquid Crystals, Second Ed., John Wiley & Sons, Inc., 2007.
3. Solid State Chemistry, A R West, Wiley 1987.
4. Modern aspect of Solid State Chemistry, C N R Rao, 1<sup>st</sup> ed., 1970.
5. Principles of Polymer Science, Bahadur P and N.V Shastry, Narosa, New Delhi, 2000.
6. Polymer Science and Engineering, D.J. Williams, Prentice Hall Inc, New Jersey, 1971.
7. Theory and Basics of Polymer Science, F.W. Billmeyer, John Wiley & Sons, NY, 1984



# ICS 505: COMPUTER AIDED DRUG DESIGN

The subject is designed to impart knowledge on the current state of the art techniques involved in computer assisted drug design

Objectives: Upon completion of this course the student should be able to

- Role of CADD in drug discovery
- Different CADD techniques and their applications
- Various strategies to design and develop new drug like molecules
- Working with molecular modeling softwares to design new drug molecules
- The *in silico* virtual screening protocols

## UNIT I

12hr

Introduction to Computer Aided Drug Design (CADD) History, different technique sand applications  
Quantitative Structure Activity Relationships: Basics History and development of QSAR: Physicochemical parameters and methods to calculate physicochemical parameters: Hammett equation and electronic parameters ( $\sigma$ ), lipophilicity effects and parameters ( $\log P$ ,  $\pi$  substituent constant), steric effects (Taft steric and MR parameters) Experimental and theoretical approaches for the determination of these physicochemical parameters Quantitative Structure Activity Relationships Deriving 2D-QSAR equations 3D-QSAR approaches and contour map analysis Statistical methods used in QSAR analysis and importance of statistical parameters

## UNIT II

12 hr

Molecular Modeling and Docking A) Molecular and Quantum Mechanics in drug design B) Energy Minimization Methods: comparison between global minimum conformation and bioactive conformation C) Molecular docking and drug receptor interactions: Rigid docking, flexible docking and extra-precision docking. Agents acting on enzymes such as DHFR, HMG-CoA reductase and HIV protease, choline esterase (AChE & BchE) Molecular Properties and Drug Design: a) Prediction and analysis of ADMET properties of new molecules and its importance in drug design. b) De novo drug design: Receptor/enzyme-interaction and its analysis, Receptor/enzyme cavity size prediction, predicting the functional components of cavities, Fragment based drug design. c) Homology modeling and generation of 3D-structure of protein

## UNIT III

10hr

Pharmacophore Mapping and Virtual Screening Concept of pharmacophore, pharmacophore mapping, identification of Pharmacophore features and Pharmacophore modeling; Conformational search used in pharmacophore mapping In Silico Drug Design and Virtual Screening Techniques Similarity based methods and Pharmacophore based screening, structure based In-silico virtual screening protocols 12

## REFERENCES:

1. Computational and structural approaches to drug discovery, Robert M Stroud and Janet.F Moore, RCS Publishers.
2. Introduction to Quantitative Drug Design by Y.C. Martin, CRC Press, Taylor & Francis group..
3. Drug Design by Ariens Volume 1 to 10, Academic Press, 1975, Elsevier Publishers.
4. Principles of Drug Design by Smith and Williams, CRC Press, Taylor & Francis.
5. The Organic Chemistry of the Drug Design and Drug action by Richard B. Silverman, Elsevier Publishers.
6. Medicinal Chemistry by Burger, Wiley Publishing Co
7. An Introduction to Medicinal Chemistry –Graham L. Patrick, Oxford University Press.
8. Wilson and Gisvold's Text book of Organic Medicinal and Pharmaceutical Chemistry, Ippincott Williams & Wilkins.
9. Comprehensive Medicinal Chemistry – Corwin and Hansch, Pergamon Publishers.
10. Computational and structural approaches to drug design edited by Robert M Stroud and Janet. F Moore

# ICP 506: SYNTHESIS OF COMPLEXES, CATALYSTS AND ESTIMATION OF ALLOYS

## Objectives

- To gain the basic analytical and technical skills to work effectively in different fields of chemistry.
  - To demonstrate the ability to synthesize and characterize compounds using published reactions, protocols, standard laboratory equipment, and modern instrumentation.
  - To learn advance techniques in gravimetric and volumetric analysis.
  - To synthesize complexes and nanocatalysts.
1. Analysis of brass–Cu gravimetrically using  $\alpha$ -Benzoinoxime & Zn complexometrically.
  2. Analysis Cu-Ni alloy.
  3. Analysis of Stainless Steel-Insoluble residue by gravimetry, Ni gravimetrically using DMG complex.
  4. Fe volumetrically using Ce(IV) & Cr(III) volumetrically by persulphateoxidation.
  5. Flame photometric determination of Na, Kmixtures.
  6. Chemical Separation Techniques
    - a. Cu(II) + Fe(II)-Cu gravimetrically as CuSCN and Fe using Ce(IV).
    - b. Cu(II) + Ni(II)-Cu gravimetrically as CuSCN and Ni using EDTA.
    - c. Fe(III) + Ca(II)-Fe gravimetrically as Fe<sub>2</sub>O<sub>3</sub> and Ca using EDTA.
    - d. Cr(III) + Fe(III)-Using EDTA by Kinetic masking method.
  7. Synthesis and characterization of potassium trioxalato chromate (III) trihydrate
  8. Solid phase synthesis of transbis glycinatocopper(II)
  9. Preparation of tris acetyl-acetoacetanato iron(II)
  10. Preparation of cis and –dichlorobis (ethylenediamine) cobalt (III)chloride.
  11. Preparation of bis-dichlorotriphenyl phosphine nickel (II)
  12. Synthesis of hexamine cobalt (II) chloride
  13. Preparation of Silver nanoparticles
  14. Preparation of ZnO nanoparticles

## Course Outcome:

Students will have the ability to:

- Think critically and analyze chemical problems.
- Present scientific and technical information resulting from laboratory experimentation in both written and oral formats.
- Work on advance techniques in gravimetric and volumetric analysis.
- Synthesize characterize complexes and nano catalysts

## References

1. G.H.Jeffrey, J.Bassette, J.Mendham and R.C.Denny, Vogel's TextBook of Quantitative Chemical Analysis ,5<sup>th</sup>Edition, Longman, 1999.
2. Vogel, "Textbook of Qualitative Inorganic Analysis", 3 Edition, ELBS. 1976.
3. D.A.Skoog and D.M.West, Fundamentals of Analytical Chemistry, IV Edition, Old Reinhold & Winston, Publication, 1982.
4. B.K. Sharma, Instrumental methods of Chemical analysis, Goel Publishing House, 24th Edition, 2005
5. Gurdeep R. Chatwal, Sham K. Anand, Instrumental Methods of Chemical Analysis, Himalaya Publication, 1979.

6. Industrial Applications of Homogeneous Catalysis, Editors: **Mortreux, A., Petit, F.** (Eds.) Springer, 1988
7. Louis S. Hegedus, Björn C. G. Söderberg Transition Metals in the Synthesis of Complex Organic Molecules Björn C. G. Söderberg, Springer 1994.
8. Nikolay Gerasimchuk, Sergiy Tyukhtenko: Inorganic Synthesis: A Manual for Laboratory Experiments Cambridge Scholars Publishing, 2021.
9. Colquhoun, H M, Holton, J, Thompson, D J, and Twigg, M V. New pathways for organic synthesis. Practical applications of transition metals. United States: N. p., 1984.

## **ICP 507: SYSTEMATIC QUALITATIVE ANALYSIS AND IDENTIFICATION OF ORGANIC COMPOUNDS**

### **Course Objectives:**

- To learn separation and estimation of binary mixture.
- To understand the identification of organic compounds by using spectroscopic technique such as  $^1\text{H-NMR}$ , FT-IR, MASS,  $^{13}\text{C-NMR}$ .

1. Separation and estimation of binary mixtures.
2. Structural elucidation of organic compounds by spectroscopic techniques.

### **Course Outcomes:**

- Students learn about separation and estimation of binary mixtures
- Students can able to identify functional groups and determine the structure of organic compounds by spectroscopic techniques.

### **References:**

1. Comprehensive practical organic chemistry: Qualitative analysis by VK Ahluwalia, Sunita Dhingra
2. More Spectroscopic Problems in Organic Chemistry-A.J. Baker et al., Hayden, 1975.
3. Spectral Problems in Organic Chemistry, Davis & Wells, Chapman & Hall, 1984.
4. Elementary Practical organic chemistry, Part 2: Quantitative organic analysis by Arthur I. Vogel, 2<sup>nd</sup> Edition, CBS Publishers and distributors, 1987.

## ICP 508: SYNTHESIS, CHARACTERIZATION AND APPLICATIONS OF POLYMERS AND COMPOSITES

### Course objectives

- To synthesize and characterize polymers and composites/nanocomposites
- To determine physical properties of polymers
- To study dye adsorption kinetics, isotherm and thermodynamics of polymers
- To evaluate water retention capacity of polymer
- To synthesize polymer nanofibers through electrospinning process and evaluate to their drug and pesticide release capacities

### List of Experiments (Any twelve experiments to be carried out)

1. Synthesis and characterization of polystyrene
2. Condensation polymerization of Nylon 6 6
3. Preparation of polysaccharide stabilized silver nanoparticles and their characterization
4. Synthesis and characterization of ZnO nanoparticle incorporated polysaccharides/polymers
5. Separation and purification of polymer quantitatively
6. Estimation of viscosity average molecular weight of polymers
7. Determination of glass transition temperature of a polymer by dilatometry
8. Determination of molecular weight of polymer by end group analysis
9. Preparation and characterization of phenol-formaldehyde resin
10. Kinetics of dye adsorption capacity of polymers
11. Dye adsorption isotherm studies of polymers
12. Thermodynamic studies of dye adsorption by polymers
13. Electrospun nanofibers of polysaccharides/polymers
14. Drug release capacities of composites of polysaccharides
15. Water absorption capacities of polymer gels and composites
16. Drug release studies of polymer nanocomposites
17. Comparison of thermal properties of polymers
18. Morphological analysis of polymers/nanocomposites

### Course outcome

- Synthesis of polymers/composites/nanocomposites and learning the physicochemical parameters
- Dye adsorption experiments using polymeric adsorbents
- Learning the electrospinning of polymers and use of thus produced fibers in drug and pesticide release

### References

1. Advanced Practical Physical Chemistry by J. B. Yadav, 5<sup>th</sup> edition, 1989.
2. Experimental Methods in Polymer Science by Toyochi Tanaka, 2000, Elsevier.
3. Polymer Synthesis and Characterization: A Laboratory Manual by S. R. Sandler, W. Karo, J. Bonesteel, and E. M. Pierce, Academic Press, New York, 1998.
4. Polymer Chemistry by S. Koltzenburg, M. Maskos and O. Nuyken, Springer, 2017.

## ICE 509: AGRICULTURE & HEALTH CARE CHEMICALS

### Course objectives

- To study classification of fertilizers, their synthesis and applications.
- To learn about characteristics of insecticides, preparations and their uses in agriculture.
- To know various methods of preparations of healthcare chemicals like soaps and detergents, perfumes.
- To learn the techniques of quality assessment and controlling measures.

### UNIT I:

12 hr.

**Fertilizers:** Introduction, Essential plant Nutrients, Classification of Essential Nutrients, Primary Nutrients, Secondary Nutrients, Micronutrients, Macronutrients, Classification of Fertilizers- Straight Fertilizers, Compound/Complex Fertilizers, Fertilizer Mixtures, Feed Stock/ Raw materials- Nitrogenous Fertilizers, Phosphatic Fertilizers, Potassic Fertilizers, Manufacture and general properties of Fertilizer products- Intermediates- Ammonia, Nitric Acid, Sulphuric Acid, Phosphoric Acid, Nitrogenous Fertilizers- Ammonium Sulphate, Ammonium Nitrate, Calcium Ammonium Nitrate, Calcium Nitrate, Ammonium Chloride, Urea, Phosphatic Fertilizers, Ground Rock Phosphate, Single Superphosphate, Triple Superphosphate, Potassic Fertilizers- Potassium Chloride (Muriate of Potash), Potassium Sulphate (Sulphate of Potash), Potassium Nitrate, Complex Fertilizers- Ammonium Phosphate Sulphate, Ammonium Phosphates, Mono Ammonium Phosphate (MAP), Di-Ammonium Phosphate (DAP), Nitrophosphates, Urea Ammonium Phosphates, NPK Complex Fertilizers, Fertilizer mixtures-Physical Mixtures, Granulated Mixtures.

### UNIT II

10 hr

**Insecticides:** Introduction, classification, Organochlorine insecticides-BHC, DDT, endosulfan, sevin, Insect pheromones, general introduction and applications in integrated pest management.  
**Repellents:** Survey & synthesis of the repellents-N,N-diethyltoluamide, 2-ethyl-1,3- hexanediol,.  
**Fungicides:** Introduction, Inorganic & organic fungicides, Systemic fungicides-types & examples.  
**Herbicides:** Introduction, study of sulfonyl ureas, Mechanism of action and toxicities of insecticides, fungicides and herbicides.

### UNIT III

10 hr

**Perfumery:** Introduction, Compounds used in perfumery and their classification, methods of preparation and importance of phenyl ethanol, Yara yara, Ionone musk ketone, musk ambrette, musk xylene, phenyl acetic acid and its esters, benzyl acetate, synthetic musks and jasmine.  
**Essential oils:** Source, constituents, isolation & uses.

### UNIT IV

10 hr

**Oils, soaps and Detergents:** Refining of edible oils, manufacturing of soaps, detergents-classification-anionic, cationic, non-ionic and amphoteric detergents, detergent builders and additives, liquid soaps. Manufacturing of fatty acids and glycerol, greases from fatty acids, turkey red oil  
**Food Analysis:** Moisture, ash, crude protein, crude fiber, fat, carbohydrate, calcium, potassium, sodium and phosphates, food adulteration-common adulteration in food, contamination of food stuffs, microscopic examination of food for adulterants, pesticide analysis in food products.

### Course Out come

- The students will be knowing about the different types of fertilizers and the synthesis and methods of use.
- The candidates will be learning about the insecticides and their uses in agriculture
- The students will be learning about the healthcare chemicals like soaps and detergents, perfumes
- They will also learn about the food quality assessment

### References

1. Statistical Quality Control, 2<sup>nd</sup> Edn., Manohar Mahajan Dampat Rai and Sons, 1995.
2. Quality management:a process improvement approach,Fryman Mark A, Cengage learning, 2002.
3. Quality Control, Paranthaman D, Tata, McGraw Hill,1987.
4. Gupta R. N. Chemical warfare and casualty management 2011
5. Vyas M. N. Safety and hazards management in chemical industries 2013.Atlantic publication.
6. Dikshith T.S.S Safety evaluation of environmental chemicals. New Age International, 1996.
7. Chemical Safety Matters-IUPAC-IPCS, Cambridge univ. Press, 1992.
8. Environmental Chemistry, A.K. Dey, Wiley Eastern.
9. Environmental Chemistry, S.K.Banerji, Prentice Hall India, 1993.
10. Chemistry of Water Treatment, S.D. Faust and O.M. Aly, Butterworths,1983.
11. Environmental chemistry, Ahluwalia V K, Anne Books India, 2008.
12. Chemistry for Environmental Engineering, Sawyer and McCarty, McGraw Hill, 1978.
13. Environmental Chemistry, I.Williams, John Wiley, 2001
14. Engineering Chemistry by Jain and Jain.
15. Industrail electrochemistry by Peltcher
16. Modern Electrochemistry, Vol I, IIA & IIB(1998) J.O.M. Bockries and A.K.N.Reddy
17. Chemical Engineers Hand Book, 8<sup>th</sup> Edn., Robert H. Perry, Mc Graw Hill, 1995.
18. Principles of Industrial Chemistry, C. A. Clausen and G. Matts.

# **IV SEMESTER**

## **INDUSTRIAL PROJECT**

### **ICP 551: Project report**

#### **Course Objective**

To learn research methodology and to form a project report on the work carried out at the Industry during IV semester.

#### **Course Outcome**

Student undergoes training at chemical industries for 4 months internship and prepare dissertation on the work carried out.

### **ICP 552: Viva –Voce examination**

#### **Course Objective**

- To present the abstract of the project work carried out during IV semester for evaluation by the examiners

#### **Course Outcome**

- The student will be acquiring hands on experience how to plan, execute and arrive at conclusions on the experiments they have to do at the industries
- This will make them job ready to be employed in a similar sectors.

#### **Program Outcome:**

- The student will be acquiring the highest level of education in chemical sciences to shape them as well informed individuals.
- The program will make significant contribution towards the development of skilled technical manpower. Thus cater to the need of growing demand of intellectual reservoir in the nation.
- The student not only acquiring fundamentals of chemistry but also hands on experience how to plan, execute and arrive at conclusions on the experiments they have to do at the industries.
- This program will make them 100% job ready to be employed in a Chemical industrial sectors.
- This will also shape them as better individuals who can venture into research, teaching and administrative career worldwide.