Department of Sciences
Manipal Academy of Higher Education
M.Sc. (Chemistry) Program
Choice Based Credit System - 2021 (CBCS - 2021)
(To be implemented from the academic year 2021-22)

Signature of Registrar

Signature of Deputy Registrar- Academics (Tech)

Signature of Coordinator-DoS

Signature of Head, Department of Chemistry

Contents

Department of Sciences
M.Sc. (Chemistry)

Rules and Regulations

Admission Procedure
Admissions are on merit based on the marks of B.Sc.

Eligibility
A pass with 50% in aggregate in B.Sc. (PCM / CBZ)

Duration
2 years (Four Semester)

Specialization offered in 2nd year
Organic Chemistry and Applied Chemistry

(Specializations can be allotted in nearly equal proportions from the intake, on merit [CGPA of 1st year] cum choice basis)

Program Educational Objectives (PEOs)
1. To prepare the post graduates in applying the knowledge in the field of chemistry to pursue higher studies and careers in chemical industries, consultancies and research institutions.

2. To enable the post graduate to exhibit critical thinking ability towards different aspects of chemistry.

3. To provide experience in planning and conducting the experiments in modern chemical laboratories with state-of-the-art facilities.

4. To instill professional attitude with ethical responsibility, effective communication skills, team work, multidisciplinary approach and train the students to apply their scientific expertise to social issues.

5. To engage in lifelong learning with knowledge of contemporary issues related to chemistry by using lab skills and techniques.

Program Outcomes (PO)
The post graduates will be able to:

1. Domain knowledge

Apply the knowledge Organic, Physical, Inorganic and Analytical chemistry to solve the scientific problems.

2. Problem analysis

Demonstrate the laboratory skills to enable them to perform both qualitative and quantitative analysis of given samples.

3. Design and Development of solution using modern techniques

Execute the designed experiment document interpret and report the data using modern tools and techniques.

4. Environment and sustainability.

Create and awareness of impact of chemistry on environment, society and development outside the scientific community.

5. Ethics

Apply ethical principle and commit to professional ethics and responsibilities of scientific practice.

6. Individual and teamwork

Perform effectively as an individual or as a team.

7. Communication

Adopt critical thinking and communicate effectively on scientific activities.

8. Life- long learning

To participate through self-paced and self-directed learning for personal development.

9. Scientific reasoning and research skills.

To inculcate the scientific temperament to recognize, analyze and formulate solution for cause and effect relationship.

10. Digital literacy

Employ information and communication technology in various learning situations.

Attendance requirements

All students are expected to attend all the lectures, tutorial and practical classes. A student with less than 75% attendance shall not be permitted to write end semester examination in that course and will be given a DT letter grade in the course.

Evaluation procedure

(a) Theory Paper: The performance of the students in each subject is evaluated using internal system of continuous assessment. The students are evaluated based on class / tutorial participation, assignment work, lab work, class tests and end-semester examinations. In all the theory papers, fifty percent weightage will be given to the in-

semester evaluation and the remaining fifty percent for end-semester evaluation. The in-semester evaluation will comprise of two sessional tests each carrying 15 marks and assignment/quiz will carry 20 marks. End semester examination will be of 50 marks. A student must obtain 40 marks altogether with minimum of 18 marks in the end semester examination. Students will be notified at the commencement of each semester about the evaluation methods being used for the subjects and the weightage given to the different assignments / activities.

(b) Lab Work: Lab work is continuously assessed, and sixty percent weightage will be given to the in-semester evaluation and the remaining forty percent for end-semester test evaluation

(c) Seminar: Written report will be evaluated for subject content, clarity of concepts, coherence, correctness, logical aspects, descriptive skills and creative writing skills. Oral presentation will be assessed for ability to express subject matter, verbal communication skills, response to questions, time management skills, and clarity of visuals on a scale exceptional (highest 1 %), excellent/outstanding (highest 5%), very good (highest 10%), good (upper 25%), fair/average (upper 50%) and poor/below average (lower 50%).

(d) Project work: Project work evaluation is done in two phases. Once in the middle of the semester and one more at the end of the semester. Evaluation is done based on the following criteria.

- Clear and concise presentation of work
- Demonstration of depth of technical understanding
- Coverage of related work; knowledge of the field
- Quality of any products or processes
- Demonstration of ability to critically analyze other work and come up with original analyses and ideas
- Any contribution to knowledge
- Demonstration of professional conduct, considering ethical issues where appropriate, and of course no evidence of plagiarism.

Relative Grading

At the end of the evaluation a letter grade in the 10-point grading system will be given to each theory / lab courses. The grade point average (GPA) is calculated at the end of each semester and CGPA at the end of each semester after the second.

Marks obtained in the in-semester and end-semester examinations (50% weightage for both) are added together and a 10-point grading system will be used to award the student with an overall letter grade for the subject. A student must obtain a minimum 40% in each subject inclusive of in-semester and end-semester examination, with minimum of 18 marks in the end semester examination, to be considered for award of the grade in that subject.

Letter Grading System

Final evaluation of subject is carried out on a TEN POINT grading system. Performance Grades and Grade Points are as shown below:

Grade	A+	A	B	C	D	E	F (Fail)
Grade Points	10	9	8	7	6	5	0

A student who earns a minimum of 5-grade points (E grade) in a subject is declared to have successfully completed the course and is deemed to be have earned the credits assigned to that course. A course successfully completed cannot be repeated.

If a student is eligible for but fails to appear in the end-semester examination, he / she will be awarded an "I" grade (incomplete) on the grade sheet. For all practical purposes, an 'I' grade is treated as "F".

If a student is not eligible to appear in the end semester examination owing to his / her not fulfilling the minimum attendance requirements, he / she will be required to discontinue the programme temporarily till such time he / she fulfills the minimum attendance requirements by re-registering for those courses in which he / she had attendance shortage at the next available opportunity.

Grade Point Average (GPA) and Cumulative Grade Point Average (CGPA)

Each subject grade is converted into a specific number of points associated with the grade. These points are weighted with the number of credits assigned to a course. The Grade Point Average (GPA) is the weighted average of Grade Points awarded to a student. The grade point average for each semester will be calculated only for those students who have passed all the courses of that semester. The weighted average of GPA's of all semesters that the student has completed at any point of time is the cumulative grade point average (CGPA) at that point of time.

CGPA up to any semester will be calculated only for those students who have passed all the courses up to that semester.

Calculation of GPA and CGPA

Example:

Courses	Credits	Letter Grade	Grade Value	Credit Value	Grade Points
Maths	3	C	7	3x7	21
Chemistry	3	B	8	3x8	24
Physics	3	A	9	3x9	27
English	2	B	8	2x8	16
Total	11				88

In this case GPA, total grade points / Credits = 88 / 11 = 8.0

Suppose the GPAs in two successive semesters are 7.0 and 8.0 with 26 and 24 respective course credits, then the

CGPA = (7.0 x 26) + (8.0 x 24) / (26 + 24) = 374 / 50 = 7.48

Generally,

$$GPA = \frac{\sum_{i=1}^{n} Ci\ Gi}{\sum_{i=1}^{n} Ci} \text{ and } CGPA = \frac{\sum_{j=1}^{N} GPAj\ x\ \sum_{i=1}^{n} Ci}{\sum_{j=1}^{N}(\sum_{i=1}^{n} Ci)}$$

where
n = number of subjects
Ci = subject credits
N = number of semesters
Gi = grade values

After the result is declared, grade cards will be issued to each student which will contain the list of courses for that semester and the grades obtained by the student, as well as GPA of that semester and CGPA up to that semester.

Re-valuation of answer papers

In case any student feels aggrieved about the evaluation, he / she shall have access to his / her answer paper in the end semester examination which may be shown to him / her by the teacher/s concerned. If the case is genuine, teacher may re-value the paper and forward a revised grade, if any, to the Head of the Department with justification for the revision. No further revision is permitted once the results are sent to the University for record.

Re-registration

Students can re-register in one or more subjects of the previous semester(s) (odd semester subjects in the odd semester only, and even semester only), provided they have F grade(s) in that subject / those subjects, by paying the prescribed fees.

Re-registration entitles the student to attend the classes (with minimum of 75% attendance requirement), and appear for the sessional tests, the end semester examinations, in the subject(s) in which they have re-registered. Re-registered candidates will have to appear for sessional tests / end-semester examinations along with the regular students.

End-Semester Examination and Make-up (Supplementary) Examination

The examinations at the end of a semester will be conducted only in the subjects of the current semester. That is, at the end of the odd-semester, examinations in the subjects of the odd-semester only will be conducted. Similarly, at the end of the even-semester, examinations will be conducted only in the subjects of the even-semester.

About 4 weeks after the conclusion of the regular examinations in the current semester subjects, there will be make-up (supplementary) examinations, before the commencement of the next semester classes. The make-up examinations will also be in

the current semester subjects only. Students who have F / I grades in one or more subjects and those who missed one or more examinations in the regular series due to serious medical reasons, are eligible to appear for the make- up examinations in the relevant subjects. The cut-off marks for conversion of marks into grades in the make-up examination will be same as those in the regular end-semester examination, in a particular subject.

However, for a student with “F” grade in any course a maximum of “C” grade will be awarded in subsequent examination irrespective of his/her performance. Student with the “I” grade with valid reasons will be allowed to retain whatever the grade he/she obtain in the make-up examinations.

Withholding of Results

Results will be withheld when a student has not paid his / her dues or when there is a case of indiscipline pending against him / her.

(These rules and regulations are subject to change / amendment from time to time, as and when need arises).

PROGRAM EDUCATION OBJECTICE (PEO)

The overall objectives of the Learning Outcomes-based Curriculum Framework (LOCF) for **M.Sc. Chemistry program are as follows.**

PEO No	Education Objective
PEO 1	To prepare the post graduates in applying the knowledge in the field of chemistry to pursue higher studies and careers in chemical industries, consultancies and research institutions.
PEO 2	To enable the post graduate to exhibit critical thinking ability towards different aspects of chemistry.
PEO 3	To provide experience in planning and conducting the experiments in modern chemical laboratories with state-of-the-art facilities.
PEO 4	To instill professional attitude with ethical responsibility, effective communication skills, team work, multidisciplinary approach and train the students to apply their scientific expertise to social issues.
PEO 5	To engage in lifelong learning with knowledge of contemporary issues related to chemistry by using lab skills and techniques.

GRADUATE ATTRIBUTES:

S No.	Attribute	Description
1	**Disciplinary Knowledge**	Knowledge of theory and practical aspects in Organic, analytical, physical and inorganic chemistry.
2	**Understanding different subsets of chemistry**	Stereochemistry, photochemistry, catalysis, spectroscopy, solid-state chemistry, organometallics, retrosynthesis, natural product chemistry.
3	**Measurable Skills and Industry-ready Professionals**	Strengthen the abilities of a learner by skills, gaining knowledge of the present scenario of pharmaceutical industry in specific and chemistry in general.
4	**Effective and Influencing communication**	Effective and Influencing communication ability to share thoughts, ideas and applied skills of communication in its various perspectives like written communication, speech communication etc.
5	**Leadership readiness/ Qualities**	To make learners fluent in multiple facets of leadership. Creating the ability & enhancing the qualities to be an efficient leader. Cultivating key characteristics in learners, to be visionary leaders who can inspire the team to greatness.
6	**Critical/ Reflective thinking & language efficiency**	Critical/ Reflective thinking ability to employ critical and reflective thinking along with the ability to create the sense of awareness of oneself and society.
7	**Technologically Efficient Professional**	Capability to use various communication technologies and ability to use various tools and techniques required for chemical industry.
8	**Ethical Awareness**	As a chemistry learner, one has to understand the importance of ethical values and its application in professional life.
9	**Lifelong Learning**	Every graduate to be converted into lifelong learner and consistently update himself or herself with current knowledge, skills and technologies. Acquiring Knowledge and creating the understanding in learners that learning will continue throughout life.
10	**Research-related Skills**	A sense of inquiry and investigation for raising relevant and contemporary questions, synthesizing and articulating.
11	**Cooperation/ Team work**	Building a team, motivating and inspiring the team members to work up with cooperation to their utmost efficiency.

Course structure

Semester	Subject code	Subject	L-T-P-C	Credits
First semester	CHM 5101	Inorganic Chemistry I	4-0-0-4	4
	CHM 5102	Organic Chemistry I	4-0-0-4	4
	CHM 5103	Physical Chemistry I	4-0-0-4	4
	CHM 5104	Spectroscopy I	4-0-0-4	4
	CHM 5105	Inorganic Chemistry Practical I	0-0-4-2	2
	CHM 5106	Organic Chemistry Practical I	0-0-4-2	2
	CHM 5107	Physical Chemistry Practical I	0-0-4-2	2
Total credits				22
Second semester	CHM 5201	Inorganic Chemistry II	4-0-0-4	4
	CHM 5202	Organic Chemistry II	4-0-0-4	4
	CHM 5203	Physical Chemistry II	4-0-0-4	4
	CHM 5204	Inorganic Chemistry Practical II	0-0-4-2	2
	CHM 5205	Organic Chemistry Practical II	0-0-4-2	2
	CHM 5206	Physical Chemistry Practical II	0-0-4-2	2
	CHM 5207	Research Methodology and Technical communication	3-0-0-3	3
Total credits				21
Third semester	CHM 6101	Spectroscopy II	4-0-0-4	4
	CHM 60XX	Elective I	3-0-0-3	3
	CHM 6051	Open elective	3-0-0-3	3
	CHM 6102	Seminar	1-0-0-1	1
	Organic Chemistry Specialization			
	CHM 6151	Advanced Organic Chemistry I	4-0-0-4	4
	CHM 6152	Organic Chemistry Practical III	0-0-6-3	3
	CHM 6153	Multistep Organic Synthesis	0-0-6-3	3
	Applied Chemistry Specialization			
	CHM 6161	Principles and Practice of Analytical Chemistry	4-0-0-4	4
	CHM 6162	Analytical Chemistry Practical	0-0-6-3	3
	CHM 6163	Applied Organic Chemistry Practical	0-0-6-3	3
Total credits				21
Fourth semester	CHM 60XX	Elective II	3-0-0-3	3
	CHM 60XX	Elective III	3-0-0-3	3
	CHM 6201	Project		6
	Organic Chemistry Specialization			
	CHM 6251	Advanced Organic Chemistry II	4-0-0-4	4
	Applied Chemistry Specialization			
	CHM 6261	Nuclear and Radiation Chemistry	4-0-0-4	4
Total credits				16
Grand Total				**80**

List of electives

CHM 6001: Materials Chemistry
CHM 6002: Industrial process and Industrial management
CHM 6003: Chemistry of Dyes and Pesticides
CHM 6004: Chemistry of Petrochemicals
CHM 6005: Applied Electrochemistry and Industrial Catalysis
CHM 6006: Green Chemistry
CHM 6007: Organometallic Cluster Chemistry
CHM 6008: Polymer Chemistry
CHM 6009: Supra molecular chemistry
CHM 6010: Solid State Chemistry and Applications
CHM 6011: Chemical Process Industries
CHM 6012: Bioorganic and Medicinal Chemistry
CHM 6013: Computational Chemistry

1st Semester

CHM 5101: Inorganic Chemistry I
[4-0-0-4]

Course Outcome:
At the end of the course students will be able to

- Explain certain key concepts in inorganic chemistry (e.g. valence bond theory, molecular orbital theory, general structural types and bonding)
- Describe the basics of analytical chemistry
- Use these concepts in problem solving
- Describe the chemistry of main group elements and transition metals

Pre-requisites:
B.Sc. Chemistry background

Syllabus

Chemical bonding:

Introduction to Bonding- Primary and Secondary bonding types, Covalent bond – V.B.T., Hybridization, V.S.E.P.R.T., M.O.T., Bond parameters, Polarity in covalent bonds, Properties of covalent compounds, Ionic bond - conditions for the formation of ionic bond, Lattice energy- Born Lande equation, Radius ratio, Ionic structures, Born-Haber cycle, Properties of ionic compounds, Covalent character in ionic bonds, Metallic bond – Metallic structures, Properties of metals, Electron sea model, Development of free electron theory to band theory of solids-metals and their properties, Semiconductors and insulators. Hydrogen bond - Types & consequences of hydrogen bonding, London forces and dipole-dipole interactions. 16

Analytical chemistry-1:

Classification of Chemical Analysis, Uncertainty in measurement, Accuracy and precision. Statistical treatment of finite samples, Least- squares method for deriving calibration of plots, Principles of sampling. Volumetric analysis- acid-base titration, redox titration, precipitation titration, Complexometric titration, Feasibility of EDTA titrations, Masking and demasking agents, Gravimetric Analysis-Practical gravimetric procedures, Mechanism of precipitate formation, Types of precipitates, Organic and inorganic precipitating reagents. 10

Chemistry of s and p block elements:

Hydrogen and its compounds, Hydrides classification, Alkali and alkaline earth metals, Solutions in non-aqueous media – ammonia. Application of crown ethers in extraction of alkali & alkaline earth metals, Boron hydrides, Metalloboranes, Carboranes, Allotropes of Carbon, Fullerenes, Oxidation states of nitrogen and their interconversion, Ring, Cage & Cluster compounds of P block elements, Silicates, Zeolites, Interhalogens: Pseudo-halogens, Synthesis, properties & applications. 12

Chemistry of Transition & Inner-transition Elements:
Transition metals- Metallic character, variable oxidations states, Stereochemistry and coordination numbers of metals, magnetic properties, measurement of magnetic moment, catalytic properties, comparison of 3d, 4d and 5d series. Lanthanides and actinides: Electronic structure, Oxidation states, Extraction and separation of lanthanides, stereochemistry, Spectral and magnetic properties of lanthanide and actinide complexes, application of Lanthanides and actinides. Comparison of f block with d-block ions. 10

References
1. J.E. Huheey, E.A. Keiter, R.L. Keiter, O. K. Medhi, *Inorganic Chemistry* 4th Edn., Pearson Education, Boston, 2008
2. D.F. Shriver, P.W. Atkins, C.H. Langford, *Inorganic Chemistry*, 3rd Edn., Oxford University Press, Oxford, 1999
3. J.D. Lee, *Concise Inorganic Chemistry*, 5th Edn., Blackwell Science Ltd., New Delhi, 2004
4. F.A. Cotton, G. Wilkinson, *Advanced Inorganic Chemistry*, 6th Edn., J. Wiley, New York, 1999
5. C.E. Housecraft, A.G. Sharpe, *Inorganic Chemistry,* 4th Edn., Prentice Hall, New Jersey , 2001

CHM 5102: Organic Chemistry I
[4-0-0-4]

Course Objectives:
At the end of the course students will be able to
- Demonstrate an understanding of organic chemistry, its principles, concepts and mechanism of organic reactions and types of reaction intermediates
- Describe the relationship between the structure of an organic molecule and its reactivity
- Explain the basic principles and concepts in the stereochemistry of organic molecules
- Organize organic chemical reactions by mechanism

Pre-requisites:
B.Sc. Chemistry background

Syllabus
Fundamental Aspects:
Brief review of structure and bonding in organic molecules. Aromaticity: Concept of aromaticity, Huckel's rule, Polygon rule, homo-aromatic, non-aromatic and anti-aromatic systems. Aromaticity in benzenoid and non-benzenoid compounds. Acids and Bases: Strength of aliphatic and aromatic acids and bases, Factors affecting strength of acids and bases, Effect of solvents on acid and base strength. Organic Reaction mechanism:

Organic reaction mechanisms involving nucleophilic substitution at saturated carbon, aromatic electrophilic, nucleophilic substitution reactions, addition reactions, elimination reactions. 12

Stereochemistry:

Introduction to stereochemistry, Representation of molecules in Fischer, Sawhorse and Newman projections including their inter-conversions, R & S notations, threo and erythro nomenclature. Principles of stereochemistry: Configurational and conformational isomerism in acyclic and cyclic compounds; stereogenicity, stereoselectivity, enantioselectivity, diastereoselectivity. Optical isomerism: Elements of symmetry, asymmetric synthesis: Cram's and Prelog's rules, 1,2-, 1,3- & 1,4-asymmetric induction. Chemo, regio and stereoselective transformations. Stereochemistry of biphenyl compounds- atropisomerism, stereochemistry of compounds containing nitrogen, sulfur and phosphorus. Winstein–Eliel equation, Curtin-Hammett principles, Cotton effect, axial haloketone rule. Geometrical isomerism: Cis-trans, E & Z, Syn & Anti isomerism. 14

Reduction and Oxidation reactions:

Reduction reactions of industrial importance, catalytic hydrogenation, metal hydride reduction, Mechanism, stoichiometry and stereochemistry of reductions with hydrides, reduction by hydride transfer reagents. Electroreduction and reductions with metals (Na, Li, Zn, Fe, Al, Mg, Sn), reductions with metal compounds, reductions with non-metal compounds, Other methods of reduction - Enzyme catalyzed reduction, Wolf-Kishner reduction, reduction with diimide and trialkysilanes. Introduction to oxidation reactions, oxidation of hydrocarbons, alcohols and ketones, oxidation with chromium and manganese compounds, per acids, periodic acids, ozone, lead tetra acetate, osmium tetroxide. 12

Organic Photochemistry:

σ and π orbitals, σ* and π* orbitals, singlet and triples states, relative energies of excited states, Jablonski diagram and quantum yield. Photo dissociation, photoreduction, photochemical isomerization and photocyclization reactions. Chemistry of excited states of organic molecules: Norrish Type - I and Type - II reactions, Di-pi methane rearrangement, Barton reaction and Photo Fries rearrangement, Paterno-Buchi reaction, Yang cyclisation, photochemistry of vision. Applications of organic dyes in energy conversion and storage. 10

References:

1. P.Y. Bruice, Organic Chemistry, Pearson Education, New Delhi, 2014
2. P.S. Kalsi, Stereochemistry- Conformation and Mechanism, New age Int, 8th edition 2015
3. E.L. Eliel, Stereochemistry of Carbon Compound, Tata McGraw Hill, New Delhi, 2013
4. J. March, Advanced Organic Chemistry-Reactions, Mechanisms and Structure, Wiley, New York, 2000
5. V.K. Ahluwalia, R.K. Parashar, Organic Reaction Mechanisms, 2nd Ed, Narosa publishing house, New Delhi, 2009

CHM 5103: Physical Chemistry I
[4-0-0-4]

Course Objectives:
At the end of the course students will be able to

- Describe electrochemical principles and applications
- Demonstrate an understanding of basic kinetic concepts, surface chemistry and catalysis
- Explain thermodynamic laws and phase rule
- Apply phase rule to simple multicomponent systems

Pre-requisites:
B.Sc. Chemistry background

Syllabus

Electrochemistry I:

Debye- Huckel theory of strong electrolytes, Debye, Huckel and Onsagar Equation- its validity, The Debye- Falkenhagen effect, The Wein effect Activity and Concentration; Activity Coefficients of Electrolytes, Variation of mean activity Coefficient with concentration- Debye- Huckel Theory of mean activity coefficients of strong electrolytes, Debye- Huckel limiting law, Determination of solute activities from solvent activities, Bjerrum's Theory of Ion Association in Electrolyte Solutions- an expression for association constant, Electro Capillary action and Electro capillary Curve, Derivation of Lippmann equation, Determination of Interfacial tension of Mercury – HCl interface by capillary rise method. The Structure of Electrified Interfaces, Concept of outer Helmholtz Plane, Quantitative thermodynamic treatment of electrified interfaces, Mathematical models for Electrified Interfaces: The Helmholtz – Perrin Model, Gouy Chapman Diffuse Charge Model and the Stern Model. 14

Chemical Kinetics:

Arrhenius equation, Activation energy- potential energy surfaces. Theories of reaction rates: kinetic theory of collision, Conventional transition state theory: (CTST)- equilibrium hypothesis, Derivation of the rate equations by the methods CTST, Thermodynamic formulation of CTST- Eyring Equation, Elementary gas phase reactions; The Lindemann Theory, Hinshelwood theory, RRK theory and RRKM theory of unimolecular gaseous reactions, Composite reactions; Rate equations for consecutive reactions- steady state treatment and rate determining step, Parallel reactions, Chain reactions with examples- Bodenstein-Lind Mechanism. Organic decompositions- thermal decomposition of ethane and acetaldehyde, Kinetics of branched chain reactions- explosion limits. Brief account of kinetics of fast reactions

Elementary Reactions in Solutions:

Transition state theory in solutions, Reactions between ions- influence of dielectric constant, Ionic strength- primary and secondary salt effect, Effect of substitutes – Hammett and Taft equation, linear free energy relationships, Isokinetic temperature,

Introduction to kinetic isotope effects and kinetics of fast reactions.
12

Surface Chemistry and Catalysis:
Uni-and bi-molecular surface reactions, Multilayer adsorption-BET equation and its application in surface area determination, Harkin`s–Jura equation and its application, Adsorption from solutions: The Gibbs adsorption isotherm. Homogeneous catalysis; General catalytic mechanisms, Equilibrium treatment Arrhenius intermediate, Steady state treatment - van't Hoff intermediate, general acid base catalysis, Mechanism of acid base catalysis, Catalytic activity and acid base strength, Enzyme catalysis- Michaelis-Menton equation, Influence of temperature and pH on enzyme catalysis, Enzyme catalysis mechanisms. Heterogeneous catalysis; Mechanism of surface reactions, Unimolecular surface reactions, Bimolecular surface reactions- Langmuir-Hinshelwood and Langmuir–Rideal mechanisms, Transition state theory of surface reactions.
12

Thermodynamics and Phase Rule:
Thermodynamic work functions, Helmholtz Free Energy, Gibbs free energy, Fundamental property relations, Maxwell's equations – thermodynamic derivation, Gibbs Helmoltz equation, Partial molar properties; Concept of chemical potential, Gibbs – Duhem equation, Duhem –Merguleus equation, Variation of chemical potential with pressure and temperature, Clapeyron–Clausius equation and its applications, Fugacity; its significance, Determination of fugacity of gas, Vant Hoff's equation, Nernst Heat Theorem and its applications, Third law of thermodynamics, Experimental verification of third law of thermodynamics, Phase rule; Application of phase rule to three component systems, Solid-liquid systems, Two salt and water system, Introduction to four component system.
10

References;
1. G. M. Barrow, *Physical Chemistry*, 7th Edn, Tata McGraw Hill, New Delhi, 2002
2. S. Glasstone, *An Introduction to Electrochemistry*, East West Press, New Delhi, 2005
3. A.W. Atkins, *Physical Chemistry ELBS*, 5th Edn, Oxford University Press, Oxford, 2000
4. K. J. Laidler, *Chemical Kinetics*, Pearson Education, 4th Edn, New Delhi, 2007
5. D.R. Crow, *Principles and applications of Electrochemistry*, 6th Edn, Chapman and Hall CRC, 2000

CHM 5104: Spectroscopy I
[4-0-0-4]

Course Objectives:
At the end of the course students will be able to
- Identify the symmetry elements, symmetry operations and the point groups of organic molecules

- Apply the group theory to interpret molecular vibrations, group theoretical selection rules for electronic transitions in different spectroscopic techniques.
- Describe the principles and instrumentation involved in MW, UV/visible, IR, Raman, Atomic Absorption and Flame Emission spectroscopic methods
- Apply the general principles to analyze and interpret spectral data

Pre-requisites:
B.Sc. Chemistry background

Syllabus

Symmetry and Group Theory:

Importance of molecular symmetry, Symmetry elements and operations - Symmetry planes, reflections, inversion center, proper/ improper axes of rotation, Products of symmetry operations- matrix representation, Classes of symmetry operations, classification of molecular point groups. Representations of groups- Representation of point groups-reducible and irreducible representation, Classification of molecules into point groups. Great orthogonality theorem (No mathematical part.). Character table. Applications of group theory. Molecular vibrations, group theoretical selection rules for electronic transitions, infra-red and Raman spectra. 10

Introduction to Spectroscopy:

Properties of electromagnetic radiation, Electromagnetic spectrum, interaction of electromagnetic radiation with matter, Components of spectrophotometer, Absorption and emission spectra of molecules. 04

Atomic Absorption Spectroscopy:

Theory of atomic spectroscopy - Origin of spectral transitions, population of energy levels, Spectral line widths, Background interferences and their correction, Instrumentation-hollow cathode lamp, atomization, flame characteristics, signal modulation, non-flame atomization techniques, double beam Atomic absorption spectrophotometer.

Flame Emission Spectroscopy - flame photometer, non-flame emission sources, comparative study & applications of AAS and AES. 10

Microwave Spectroscopy:

Theory of microwave spectroscopy - rotational spectra of rigid and non-rigid diatomic molecules and polyatomic molecules, intensity of spectral lines, isotope effects, Stark effect, instrumentation and applications. 04

IR Spectroscopy:

Theory of IR spectroscopy - Vibrational & vibrational-rotational spectra of diatomic molecules, modes of vibration in poly atomic molecules, Factors influencing vibrational frequencies, instrumentation, Solid, liquid and gaseous sampling techniques, double beam IR spectrophotometer, FTIR. Identification of functional groups of organic compounds, correlation charts, other applications in organic chemistry. 10

Raman Spectroscopy:
Principles of Raman effect, Quantum & classical theories of Raman effect, Rotational & Vibrational Raman spectra, Instrumentation, laser Raman spectrometer. Applications in organic chemistry, difference between IR & Raman spectra, advantages & disadvantages of Raman spectroscopy over IR spectroscopy. 04

UV- Visible Spectroscopy:
Laws of absorption of light- Beer's &Lambert's law, limitations of Beer's law, Types of electronic transitions in organic molecules, Chromophores & oxochromes, Bathochromic & hypsochromic shifts, Charge transfer transitions, Instrumentation & sampling, Solvent effects, Applications of electronic spectroscopy in the elucidation of structure of organic compounds- Woodward Feiser rules, Quantitative analysis, Photoelectron spectroscopy-basic principles, measurement techniques and applications. 06

References
1. Skoog, Holler, Nieman, *Principles of Instrumental Analysis*, 5th Edn, Thomson Brooks/Cole, 2006
2. Gurdeep R. Chatwal, Sham K. Anand, *Instrumental Methods of Chemical Analysis*, 5th Edn, Himalaya Publishing House, 2007
3. C.N. Banwell, E.M. McCash, *Fundamentals of Molecular Spectroscopy*, Tata McGraw Hill, New Delhi, 2001
4. R.M. Silverstein, *Spectrometric Identification of Organic Compounds*, John Wiley & Sons, New York, 2005
5. W. Kemp, *Organic Spectroscopy*, 3rd Edn, ELBS, Hampshire, 2001
6. G. Aruldhas, *Molecular Structure and Spectroscopy*, Prentice Hall, New Delhi, 2001

CHM 5105: Inorganic Chemistry Practical I
[0-0-4-2]

Course Objectives:
At the end of the course students will be able to
- Explain the principles of gravimetric and volumetric analysis
- Use the skills developed in the lab course in inorganic quantitative analysis
- Demonstrate quantitative analysis skill of certain ores, alloys and pigments
- Discuss some key introductory concepts of inorganic chemistry in quantitative analysis

Pre-requisites:
B.Sc. Chemistry background

List of experiments
1. Analysis of pyrolusite-insoluble residue gravimetrically and manganese content by oxalate method.
2. Determination of manganese by gravimetric analysis.

3. Colorimetric determination of Iron by thiocyanate method and gravimetric determination of lead.
4. Colorimetric determination of Copper by aqueous ammonia and gravimetric determination of nickel.
5. Determination of iodide by KIO3 and gravimetric determination of thiocyanate.
6. Analysis of Hematite - insoluble residue gravimetrically and Iron determination by volumetric method.
7. Analysis of Dolomite-insoluble residue gravimetrically and Ca, Mg by complexometric method.
8. Analysis of stainless steel-insoluble residue gravimetrically and determination of Ni by gravimetric and Fe by volumetric methods.
9. Analysis of brass-determination of copper gravimetrically and Zinc complexometric method.
10. Analysis of white lead – determination of lead gravimetrically and volumetrically by EDTA method.

Reference:

1. Svehla and Sivasankar, Vogel's Qualitative Inorganic Analysis, 7th Edn., Pearson Education India, 2012
2. J. Mendham, R. C. Denney, J. D. Barnes, M. Thomas, Vogel's textbook of quantitative chemical analysis, 6th Edn., Prentice Hall, 2000.

CHM 5106: Organic Chemistry Practical I

[0-0-4-2]

Course Objectives:

At the end of this course students should be able to

- Perform synthetic reactions, work-ups and purifications
- Measure and report relevant physical properties of prepared compounds

Pre-requisites:

B.Sc. Chemistry background

List of experiments

1. Synthesis of adipic acid from cyclohexanol.
2. Oxidation of benzaldehyde using potassium permanganate.
3. Preparation dibenzylidineacetone from benzaldehyde.
4. Synthesis of benzpinacol from benzophenone.
5. Reduction of benzophenone to benzohydrol.
6. Preparation of diazoaminobenzene from aniline.
7. Synthesis of aryloxy acetic acid from p-cresol.
8. Preparation of coumarin derivative from resorcinol.
9. Nitration of acetanilide to p-nitroacetanilide.
10. Hydrolysis of p-nitroacetanilide to p-nitroaniline.

References:

1. A.I. Vogel, A Text Book of Practical Organic Chemistry, Pearson Education; 5 edition (2003).
2. F.G. Mann, B.C. Saunders, Practical Organic Chemistry, Pearson Education India; 4th edition (2009).

CHM 5107: Physical Chemistry Practical I

[0-0-4-2]

Course Objectives:

At the end of this course students should be able to

- Describe basic procedures and techniques used in physical chemistry in acquiring data
- Perform experiments in physical chemistry involving conductometry, potentiometry, refractometry and kinetics
- Apply the principles of kinetics and electrochemistry in the lecture courses in some illustrative experiments

Pre-requisites:

B.Sc. Chemistry background

List of experiments

1. Conductometric titrations: i) Weak acid vs strong base ii) Mixture of strong and weak acid vs strong base iii) Strong acid vs weak base.
2. Kinetics of inversion of sucrose using polarimeter in HCl and H2SO4 media and determination of their relative strengths.
3. Determination of percentage composition of binary mixture by using refractometer.
4. Determination of formal potential of Fe2+/Fe3+ system using three different oxidants by potentiometric method.
5. Determination of pH of buffer and pKa of acids- using pH meter.
6. Potentiometric precipitation titrations of potassium halides by using standard silver nitrate solution.
7. Kinetics of acid catalyzed hydrolysis of an ester.
8. Determination of distribution coefficient of iodine in carbon tetrachloride and water system.
9. Potentiometric determination of dissociation constants of weak acids.
10. Verification of Nernst equation.

References:

1. B. Yadav, Advanced Practical Physical Chemistry, Krishna Prakashan Media (P) Ltd, 2015
2. V.D. Athawala, P. Mathur, Experimental Physical Chemistry, New Age International, 2001
3. B. Viswanathan, P.S. Raghavan, Practical Physical Chemistry, Viva Books Pvt. Ltd, 2014
4. B.P. Levitt, Findlay's Practical Physical Chemistry, 9th Edn, Longman, 2000

2nd Semester

CHM 5201: Inorganic Chemistry II
[4-0-0-4]

Course Objectives:
At the end of the course students will be able to

- Explain the concepts in co-ordination and solid state chemistry
- Understand the principles of bio-inorganic chemistry and enzyme catalysis
- Comprehend the principles of thermal analysis and chromatographic techniques

Pre-requisites:
CHM 5101

Syllabus

Co-ordination Chemistry:

Coordination numbers and structures of complexes, Concept and scope of ligand fields, Effect of ligand field-octahedral and tetrahedral, Isomerism in coordination compounds, MOT of complexes, Electronic spectra of complexes, Transition metal magneto chemistry, Spectrochemical series, Nephelauxetic effect, John-Teller theory, Stability constants of complex ions, Factors affecting the solution stability, Structure of co-ordination complexes with co-ordinate number 1,2,3 and 4. Uses of coordination compounds. 14
Kinetics

Bioinorganic Chemistry:

Principles, Ligands of biological interest, Metalloproteins, Storage and transport of metals, Electron transfer. Dioxygen transport, Photosynthesis, Dinitrogen fixation in nature and biological models, Metals in medicine, Metal toxicity, Enzyme catalysis, Hemoglobin, Carboxypeptidase, Carbonic anhydrase, Ferredoxins, Cytochromes, Cyano-cobalamin, Chlorophyll. 10

Solid State Chemistry:

Brief review of crystal systems, space groups and crystal structures. Methods of characterizing crystal structure - Powder x-ray diffraction, electron and neutron diffraction; Thermal analysis, Microscopy and spectroscopy as tools of characterization. 10

Analytical Chemistry-II:

Electro gravimetry, Principles, instrumentation and applications. Thermal analysis techniques: TGA, DTA, Chromatographic techniques: Classification, Experimental techniques, advantages, disadvantages of thin layer chromatography, liquid chromatography, HPLC, Gas chromatography and Gel chromatography, Ion exchange chromatography. Solvent extraction: Principles, Extraction techniques and applications. 14

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References:

1. B. Douglas, D. McDaniel, J. Alexander, *Concepts and Models of Inorganic Chemistry*, John Wiley, New York, 2000
2. J.E. Huheey, E.A. Keiter, R.L. Keiter, O. K. Medhi, *Inorganic Chemistry*, 4th Edn.,Pearson Education, New Delhi, 2006
3. R.M. Roat, Malone, *Bioinorganic Chemistry*. A Short Course, 2nd Edn, Wiely New Jersey, 2007
4. Skoog, Holler, Nieman, Principle of Instrumental Analysis,5th Edn, Thomas Asia ptc. Ltd, 2004.
5. G.R. Chatwal and S. Anand, Instrumental Methods of Chemical Analysis, 5th Ed., Himalaya Publishing House, 2014

CHM 5202: Organic Chemistry II

[4-0-0-4]

Course Objectives:

At the end of the course students will be able to

- Demonstrate an understanding of pericyclic reactions and predicts their mechanisms using FMO and Woodward-Hoffman correlation diagram.
- Describe various photochemical reactions focusing selected photochemical named reactions.
- Explain the synthetic utilities of various reagents for organic transformations and to describe their selectivity
- Predict the reaction mechanism and suggest the viable synthetic choices.

Pre-requisites:

CHM 5102

Syllabus

Pericyclic Reactions:

Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl systems, Classification of Pericyclic reactions, Woodward-Hoffmann correlation diagram and FMO approach, Electrocyclic reactions: Introduction, Con-rotatory and dis-rotatory process, 4n and 4n+2 systems, Cycloaddition reaction: Suprafacial and antarafacial addition using 4n and 4n+2 systems, Sigmatropic reactions: Suprafacial and antarafacial shift of H and methyl group during [1,3] & [1,5] - sigmatropic shifts, Claisen, Cope, Oxy-Cope and Aza-Cope rearrangements. 12

Reagents in Organic Synthesis-I:

Sharpless asymmetric epoxidation, DDQ, Dioxiranes, Selenium dioxide, DMSO with either Ac_2O or oxalyl chloride, Dess-Martin reagent. Synthesis involving phase transfer catalysis (PTC), Baylis-Hillman reaction, Henry reaction, Nef reaction, Kulinkovich reaction, Ritter reaction, Sakurai reaction, Tishchenko reaction and Ugi reaction. Brook rearrangement; Tebbe olefination. Metal mediated C-C and C-X coupling reactions:

Palladium catalyzed cross coupling reactions, Ullmann coupling reactions, directed ortho metalation. 12

Transition Metal Organometallics:

Definitions, Importance of organometallic compounds as reagents, additives and catalysts, Classification of organometallic compounds, Types of ligands, Heptacity, Preparation, reactions and structure of ferrocene, metal carbonyls and pi-bonded organic ligands such as alkenes, alkynes, allyls, and arenes. Metal carbenes and carbynes; synthesis, reactions, nature of bond and structural characteristics. Transition metal hydrides; synthetic routes, structure, reactivity and applications. Preparative methods, nature of bonding, structural features of olefinic, acetylenic, allylic, butadiene, cyclobutadiene, η^5- cyclopentadienyl, η^6- benzene, cycloheptatriene, cyclooctatetraene complexes. Metal alkyls; decomposition pathways, stable alkyls, preparation, properties and reactions. Important reactions relating to nucleophilic and electrophilic attack on ligands. Fluxional isomerism in olefin, allyl, dienyl and cyclopentadienyl complexes. 14

Main- group Organometallics:

General methods of preparation of main group organometallics: Oxidative addition, transmetallation, metal-halogen exchange, metal-hydrogen exchange reactions. Properties, reactivity as nucleophile, base, reductor. Structures – sigma, 3c-2e bonds. Preparation, properties and applications of organometallic compounds of Li, Mg, Si, B, Al, and Sn, Formation of C-C single bonds using organolithium/magnesium/zinc reagents. 10

References

1. R.O.C. Norman, J.M. Coxon, *Principles of Organic Synthesis*, 3rd Edn., CRC Press, New York, 2017
2. Caruthers, *Some Modern Methods of Organic Synthesis*, Cambridge University Press, Cambridge, 1999
3. O.L. Chapman, *Organic Photochemistry*. Vol I & II., Marcel Decker, New York, 1998
4. P.Y. Bruice , *Organic Chemistry*, Pearson Education, New Delhi, 2002.
5. G.O. Spessard, G.L. Miessler. Organometallic Chemistry. Prentice-Hall, New Jersey, 2009.
6. R.H. Crabtree, *Organometallic Chemistry of Transition Metals*, 3rd Edn., Wiley, New York, 2000
7. C. Elschenbroich, A. Salzer, Organometallics: A Concise Introduction, VCH Publishers, Weinheim, 2006.
8. R.C. Mehrotra, A. singh, *Organometallic Chemistry*, 2nd edition, New age Int. 2000

CHM 5203: Physical Chemistry II

[4-0-0-4]

Course Objectives:

At the end of the course students will be able to

- Describe the applications of galvanic cell and electrolytic cells
- Explain the quantum mechanical treatment of simple molecules

- Correlate molecular structure and molecular properties using quantum chemistry principles

Pre-requisites:
CHM 5103

Syllabus

Electro-chemistry II:

Galvanic cells as energy sources: Primary and secondary cells, Brief discussion on lead storage cell and Ni-Cd cell, Lithium primary and secondary cells, Fuel cells: classification, construction and working of alkaline fuel cell and polymer electrolyte fuel cell
Electrolytic cells: decomposition potential, polarization and over voltage. Electroplating: need and factors affecting electro deposit. Brief discussion on electroplating of Cr. Electro-less plating: principles, electro-less plating of Cu 08

Quantum Chemistry:

Review of basic mathematics, Origin and development of quantum chemistry: black body radiation, dual nature of light, de-Broglie hypothesis, dual nature of particles, Heisenberg's uncertainty principle, Concept of particle wave: Schrodinger wave function and its physical significance, conditions for acceptable wave function, conditions for normalization and orthogonality, Quantum mechanical formalization; Operators, Eigen values and Eigen functions, Basic postulates of quantum mechanics, Derivation of time independent Schrodinger wave equation, Solution of Schrodinger wave equation for exactly solvable problems such as particle in a box (1D and 3D), Harmonic oscillator (comparison between classical and quantum mechanical treatment), Quantum mechanical tunneling effect, Particle rotating in a ring, sphere, Rigid rotor.(solutions for θ,ϕ equations) Circular harmonics 14

Atomic Structure:

Structure of hydrogen and hydrogen like atoms (separation of r,θ,ϕ equations and their solutions), Quantum numbers and their characteristics, Orbital diagram. Spherical harmonics Need of approximation methods, Method of variation and perturbation, Application of variation method to H & He atoms- Secular equations and secular determinants, Structure of many electron systems/atoms, Structure of multielectron atoms - Self consistent field approximation and Hartree Fock Self consistent field approximation, Slater type orbitals: Slater rules, Angular momentum (commutations, relations, operators), Term symbols, Russell-Saunders terms and Coupling schemes. 14

Theoretical Approach to Chemical Bonding:

Theory of chemical bonding of diatomic molecules, Born Oppenheimer approximation, MOT and VBT for hydrogen molecular ion, Theory of chemical bonding of poly atomic molecules- ab initio method, Semi empirical method, Empirical method; Huckel molecular orbital theory of linear conjugated systems (ethene, allyl & butadiene systems) and aromatic molecules (benzene as an example). Calculation of delocalization energies, Bond order and charge density. 12

References:
1. I. N. Levine, *Quantum Chemistry*, 5th Edn, Allwyn and Bacon, Boston, 2000
2. P.W. Atkins, *Molecular Quantum Chemistry Mechanics*, 3rd Edn, Oxford University Press, Oxford, 2001
3. A.K. Chandra, *Introductory Quantum Chemistry*, Tata McGraw Hill, New Delhi, 2000
4. R.K. Prasad, *Quantum Chemistry*, New Age International Publication, New Delhi, 4th Edn., 2010
5. A. Skoog, D.M.West, F.J. Holler, S.R.Crouch, *Fundamentals of Analytical Chemistry*, 8th Edn, Thomson Brooks Cole, Belmont, 2008

CHM 5204: Inorganic Chemistry Practical II
[0-0-4-2]

Course Objectives:
At the end of the course students will be able to
- Describe certain key inorganic concepts involved in qualitative analysis
- Demonstrate semi micro analysis skill of mixtures of inorganic salts

Pre-requisites:
B.Sc. Chemistry background

List of experiments
Semi-micro qualitative inorganic analysis of mixtures of inorganic salts containing four cations and two anions (two less common cations like Tl, W, Mo, V, Zr, Th, U, Ce, Ti and Li and anions such as phosphate, borate and fluoride to be included).
Semi-micro qualitative inorganic analysis- Experiments 1-10.

References:
1. A.I. Vogel, A text book of Inorganic qualitative Analysis, ELBS, 2004
2. J. Mendham, R. C. Danney, J. D. Barnes, M. Thomas. Vogel's Textbook of Quantitative Chemical Analysis, Pearson Education, 2000

CHM 5205: Organic Chemistry Practical II
[0-0-4-2]

Course Objectives:
At the end of the course students will be able to
- Separate and identify the components present in the given unknown organic mixture through physical properties, chemical tests and derivative preparation
- Perform semi-micro qualitative organic analysis of simple mixtures

Pre-requisites:
B.Sc. Chemistry background

List of experiments
Separation of binary and ternary mixtures of organic compounds, Organic mixtures containing aromatic hydrocarbons, carboxylic acids, phenols, amines, nitro compounds, amides, carbonyl compounds and halogenated compounds.
Semi-micro qualitative organic analysis: Expt. 1 – 10.

References:
1. A.I. Vogel, A Text Book of Practical Organic Chemistry, Pearson Education; 5 edn., 2003.
2. F.G. Mann, B.C. Saunders, Practical Organic Chemistry, Pearson Education India; 4 edn.,2009.

CHM 5206: Physical Chemistry Practical II
[0-0-4-2]

Course Objectives:
At the end of the course students will be able to
- Preform physiochemical measures including solubility product, stability constant, rate constant and molecular weight
- Interpret scientific information and experimental data in the determination of several parameters and physical constants

Pre-requisites:
B.Sc. Chemistry background

List of experiments
1. Determination of rate constant of the reaction between potassium persulfate and potassium iodide by colorimetric measurements.
2. Determination of the solubility product of silver chloride using a galvanic cell and a concentration cell.
3. Determination of energy of activation and thermodynamic parameters for the acid catalyzed hydrolysis of methyl acetate.
4. Determination of percentage composition of a binary mixture by surface tension method.
5. Determination of density, viscosity and their variation with temperature of an organic liquid.
6. Verification of Freunlich's and Langmuir adsorption isotherms.
7. Determination of partial molar volumes of (a) Salts – water and (b) alcohol – water (methanol & ethanol) systems by density method.
8. Determination of dissociation constant of formic acid, acetic acid and monochloroacetic acid by conductometric method.
9. Influence of ionic strength on the rate constant of the reaction between potassium persulfate and potassium iodide.
10. Determination of molecular weight of the polymer by viscosity measurements.

References

1. J.B. Yadav, Advanced Practical Physical Chemsitry, Goel Publishing House, 27th Edn., 2008
2. V.B. Athawale, P. Mathur, Experimental Physical Chemisty, New Age International, 2008
3. G.R. Chatwal, S. M. Anand, Instrumental Methods of Chemical Analysis, 5th Edn., Himalaya Publishing House., 2009
4. B.P. Levitt, Findlay's Practical Physical Chemistry, 9th Edn, Longman, 2003

CHM 5207: Research Methodology and Technical Communication
[3-0-0-3]

Course Objectives:
At the end of the course students will be able to

- Explain certain key concepts in research
- Use these concepts in problem solving and data analysis
- Practice these concepts in writing thesis and research communications

Pre-requisites:
B.Sc. Chemistry background

Syllabus

Introduction to Research methodology:

Types of research, Significance of research, Research framework, Case study method, Experimental method, Sources of data, Data collection using questionnaire, interviewing, and experimentation. Components, selection and formulation of a research problem, Objectives of formulation, and Criteria of a good research problem. Criterion for hypothesis construction, Nature of hypothesis, Characteristics and Types of hypothesis, Procedure for hypothesis testing.
Introduction to Chemical research: Type of chemical research, Research framework as applied to chemical sciences, Theoretical and experimental approaches, Chemistry and interdisciplinary research. 12

Experimental methods and data analysis in chemical Sciences:

Measurement and Scaling Techniques, Methods of Data Collection and analysis, standard deviation, coefficient of variation, Student t-test, Processing & Analysis of Data, Presentation of Figures and Tables, Interpretation of spectral data (Focus on presentation of data and their analysis) Thermal methods of analysis, Electroanalytical methods, Miscellaneous techniques- Illustrative examples by case study method. 12

Literature Review and Journal communications:

Importance of literature review. Performance of literature review, Sources of chemical literature, identification of research gap, defining scope and objectives of the research problem, Styles of referencing.

Preparation of conference presentations (Oral and Poster) by case study method, Effective Presentation; Journal communication: Type of articles, Journal quality criteria-Impact factor and article level matrices, Importance of copyrights, Ethics in research and publishing: Plagiarism and related issues-Case studies, Criteria for authorship, Preparation of dissertation. 12

References:

1. R. Kumar, Research Methodology; A Step-by-Step Guide for Beginners, SAGE 2005
2. G. R. Marczyk, D. De Matteo and D. Festinger, Essentials of Research Design and Methodology, John Wiley &Sons 2004
3. S. C. Sinha, A. K. Dhiman, Research Methodology, Vedam Books 2006
4. C. R. Kothari, Research Methodology; Methods & Techniques, New age international publishers, New Delhi 2008.
5. T. Chakraborty, L. Ledwani, Research Methodology in Chemical Sciences Experimental and Theoretical Approach, CRC Press, 2016.

3rd Semester

CHM 6101: Spectroscopy II
[4-0-0-4]

Course Objectives:
At the end of the course students will be able to

- Explain the principles, concepts and applications of 1H and 13C NMR spectroscopic techniques
- Explain the principles, concepts and applications of NQR, ESR, Mossbauer spectroscopic techniques
- Explain the principles, concepts and applications of Mass spectrometry
- Apply these analytical methods in elucidating the structure of organic molecules

Pre-requisites:
CHM 5104

Syllabus

Proton NMR Spectroscopy:

General principles, Quantum & Classical theories, NMR spectrum- number & intensity of peaks, Chemical shift & its measurements, Factors affecting chemical shifts, Solvents used in NMR, Spin-spin coupling, Coupling constant, Chemical & magnetic equivalence in NMR, chemical exchange, factors affecting coupling constant, Karplus relationships, non- first order spectra, simplification of complex proton NMR spectra, Instrumentation- Continues wave NMR spectrometer, FT-NMR, applications- correlation tables, Elucidation of structure of organic molecules. 14

13C NMR Spectroscopy:

^{13}C nucleus, recording of spectra, general aspects of ^{13}C NMR spectrum- resolution, Proton decoupling, off resonance proton decoupling, line intensity, chemical shifts equivalence, correlation data, factors affecting carbon chemical shifts and its corrections, spin-spin coupling and double irradiation, INDOR, SPI, NOE, variable temperature NMR, DEPT spectra, 2D NMR, COSY, MRI, CIDNP, Heteronuclear coupling.
^{19}F, ^{31}P, ^{14}N, ^{15}N, and ^{17}O NMR –general aspects and examples. 10

NQR Spectroscopy:

Quadrupole nucleus, Principle of NQR, Transitions for axially & non-axially symmetric symmetric systems, Instrumentation and applications. 04

ESR Spectroscopy:

Basic principles, Total Hamiltonian, Hyperfine structure, ESR spectra of molecules and free radicals, The ‘g’ factor, systems in triplet states, ESR of transition metal ions, Techniques and instrumentation of ESR, applications, ENDOR, ELDOR.

Mossbauer Spectroscopy:

Theory - recoilless absorption & emission, isomer shift, Quadrupole interaction, Magnetic hyperfine interaction, Experimental techniques, Applications. 06

Mass Spectrometry:

Basic principles, Instrumentation-Ion source, Mass analyzer, Detector, Isotopic abundance, Molecular ion, Meta stable ion, Calculation of meta stable ion m/z values, Fragmentation patterns. Fragmentation associated with functional groups, Chemical ionization, Electrospray ionization, Field ionization and field desorption. Desorption by lasers, plasmas, atoms and ions- LD, LIMA, PD, SIMS and FAB, GC-MS & LC-MS techniques, Isotope substitution, Time-of-flight MS, Quadrupole MS, FTMS, Applications, Mass spectra of organic compounds, Trace gas analysis, Problems based on joint application of several spectroscopic techniques. 14

References:

1. C.N. Banwell, E.M. McCash, *Fundamentals of Molecular Spectroscopy*, Tata McGraw Hill, New Delhi, 5th Edition, 2013
2. R.M. Silverstein, *Spectrometric Identification of Organic Compounds*, John Wiley & Sons, New York, 8th Edition, Wiley, 2014.
3. W. Kemp, *Organic Spectroscopy*, 3rd Edn, ELBS, Hampshire, 2017
4. G. Aruldhas, *Molecular Structure and Spectroscopy*, Prentice Hall, New Delhi, 2001

CHM 60XX: Elective I

[3-0-0-3]

The department will offer three papers from the basket of electives. The students has to give their preferences. If the number of students opting for a particular elective is less than 5, such students' second preference will be considered.

CHM 6051: Open elective

(Offered to students of other M.Sc. program)

Chemistry in Everyday Life

Objectives

- visualise the importance of Chemistry in daily life
- know about artificial sweetening agents and food preservatives
- discuss the chemistry of dyes, cleansing agents and polymers
- describe the basis of classification of drugs
- explain the significance of biomolecules, oils and fats
- describe the importance of chemicals in agriculture

Chemicals in food:

Artificial sweeteners- Aspartame, Alitame, Sucralose. Food preservatives - Benzoates, propionates, sorbates, disulphites. Flavors - vanillin, alkyl esters (fruit flavors), monosodium glutamate. Artificial food colorants - coal tar dyes and non-permitted colours and metallic salts. Food adulterants - Types of adulterants, common food adulterants. 2 h

Chemicals in dyeing:

Dyes- colour and constitution, classification of dyes, General study on azo dyes, mordant dyes, vat dyes, indigo dyes, optical brighteners. 3 h

Chemicals as drugs:
Classification of drugs, drug-target interaction, therapeutic action of different classes of drugs - antacids, antihistamines, tranquilizers, analgesics, antimicrobials, anthelmintics, antimalarials, antifertility drugs. 3 h

Chemicals in water treatment:
Hydrologic cycle, criteria and standards of water quality-safe drinking water. Public health significance and measurement of water quality parameters- Colour, turbidity, total solids, acidity alkalinity, hardness, sulphate, flouride, phosphate, nitrite, nitrate, BOD and COD Water purification for drinking and industrial purposes Hard water - problems, softening techniques. Waste treatment - solid and liquid industrial wastes. Sewage and industrial effluent treatment. 4 h

Chemicals as cleansing agents:
Soaps- Types with examples, cleansing action. Synthetic detergents- Types with examples, cleansing action. 2 h

Chemicals in agriculture:
Composition of soil- inorganic and organic components in soil-micro and macronutrients Fertilizers - classification with examples, straight and compound fertilizers, Fertilizer mixtures, general properties and functions of some common fertilizers like urea, DAP etc. Pesticides - classification with examples, properties, function and environmental effects Insecticides - classification with examples, insect repellents. 6 h

Chemistry of biomolecules
Carbohydrates: classification with examples, functions, structure of mono, di and polysaccharides - glucose, fructose, sucrose, lactose, starch and cellulose. Proteins: amino acids, polypeptides, proteins - classification with examples and function. Vitamins: sources, classification with examples, functions 6 h

Chemistry of energy in daily use:
Principles and applications of primary & secondary batteries and fuel cells, photovoltaic cells, future energy storage. Corrosion- types and prevention. 4 h

Chemistry of polymers:
Classification of polymers, Typical examples. Applications in textiles, electronic, automobile, aeronautic, medical fields, plastic waste management, bio-friendly polymers 2 h

Chemistry of oils and fats:
Classification, edible oils and fats, composition, properties, rancidity. 2 h

Air Pollution:

Air pollutants, prevention and control, greenhouse gases, acid rain, ozone hole and CFC's, photochemical smog and PAN. 2 h

References

1. B. K. Sharma: introduction to Industrial Chemistry, Goel Publishing, Meerut (1998)
2. Medicinal Chemistry by Ashutosh Kar.
3. Drugs and Pharmaceutical Sciences Series, Marcel Dekker, Vol. II, INC, New York.
4. Chemical Analysis of Foods - H.E.Cox and pearson.
5. Foods: Facts and Principles. N. Shakuntala Manay and S. Swamy, 4th ed. New Age International

CHM 6102: Seminar

[1-0-0-1]

The student must present a topic of interest (not covered in the syllabus). All other students must attend the seminar and get benefit. The seminar will be conducted on a specific date, as notified by the seminar coordinator.

Organic Chemistry Specialization

CHM 6151: Advanced Organic Chemistry I

[4-0-0-4]

Course Objectives:

At the end of the course students will be able to

- Explain the organic chemistry concepts and principles in rearrangement and named reactions
- Write the mechanism of various organic reactions
- Describe the synthetic methods of certain organic compounds
- Explain the disconnection approach, principles and techniques used in retrosynthetic analysis
- Apply organometallic chemistry to synthesize simple organic molecules and polymers

Pre-requisites:

CHM 5102

Syllabus

Rearrangement Reactions and reactive intermediates:

Molecular rearrangements: Nucleophilic, electrophilic, free radical rearrangements. Intermolecular and intramolecular migrations. Wagner-Meerwein, Pinacol-pinacolone, Benzyl-benzilic acid, Fries, Wolf, Fevorsky, Neber, Sommlet-Hauser, Hoffmann, Beckmann, Losen, Curtis, Schmidt and Benzedine rearrangements. Mechanistic classification, Nucleophiles and electrophiles, movement of electrons and rate of reaction.

Generation stability and reactivity of classical and non-classical carbonium ions, carbanions, carbenes, free radicals, nitrenes, benzynes and arynes 10

Named Reactions:

Mechanism, stereochemistry and applications of named reactions, Aldol, Perkin, Reimer-Tiemann, Reformatsky, Diels-Alder, Friedal-Crafts, Wittig reactions, Michael addition, Oppenaur oxidation, Clemenson, Wolf-Kishner, Meerwein-Varley-Pondorf and Birch reductions, Mannich reactions, Ene reaction, Bayer-Villiger oxidation reaction Suzuki coupling reaction Grignard reaction. 10

Retrosynthetic Analysis:

Introduction to disconnection approach, principles and techniques used for disconnections, Synthons and synthetic equivalents, Interconversion of functional groups, One group C-X disconnections, and two group C-X disconnections, Chemoselectivity. Disconnection strategies in 1,1 1,2 1,3 1,4 1,5 and 1,6-difunctionalised compounds, Natural and reversed polarity (umpolung), umpolung strategies, donor and acceptor synthons.

Protecting groups: Principle of protection of hydroxyl, amino, carboxylic and carbonyl groups. Amine and alcohol synthesis. Approach to cyclic systems and reconnection strategies. Alkene synthesis. General strategies of disconnection. Stereo and regio selectivity, D-A reactions. Heterocyclic synthesis: 3, 4, 5, 6-membered heterocycles, fused heterocycles, Rearrangement in synthesis. Retrosynthetic analysis of industrially important compounds. 16

Applications of Organometalics in Organic Chemistry:

16- and 18-electron rules, Unique reactions in organometallic chemistry-oxidative addition, reductive elimination, migratory insertion and elimination reactions, ligand substitution reactions, activation of ligands for external attack, carbonylation and decarbonylation, nucleophilic attack on coordinated ligands, ligand coordination and dissociation reductive coupling, Homogeneous catalysis; hydrogenation, hydrosilation, hydrocyanation, isomerization of olefins, Immobilisation of homogeneous hydrogenation catalysts, Hydroformylation mechanism, Monsanto acetic acid process. Wacker process, Olefin metathesis, Ziegler-Natta polymerization, Fischer -Tropsch reaction, Water Gas shift reactions, fluxionality in organometallic compounds, Organometallic compounds as drugs, radiopharmaceuticals, tracers, ionophores and sensors. 12

References:

1. S. Warren, P. Wyatt, *Organic Synthesis: The Disconnection Approach*, John Wiley & Sons, New York, 2008.
2. J. Clayden, *Organic Chemistry,* Oxford University Press, 2000.
3. V.K. Ahluwalia and R.K. Parashar, *Organic Reaction Mechanisms*, 2nd Edn., Narosa publishing house, New Delhi, 2009.
4. R. Bruckner, *Advanced Organic Chemistry- Reaction Mechanisms*, Academic press, San Diego, 2005.
5. D. Astruc, *Organometallic Chemistry and Catalysis*, Springer, Berlin, 2007.

CHM 6152: Organic Chemistry Practical III
[0-0-4-2]

Course Objectives:
At the end of the course students will be able to

- Quantify the percentage of organic compounds in a given sample
- Develop the skill in extracting the ingredients from the plant source
- Separate the mixtures using chromatographic techniques

Pre-requisites:
B.Sc. Chemistry background

(Any ten experiments to be performed)
List of experiments
1. Estimation of Amino acid
2. Estimation of Phenol
3. Hydroxy group by acetylation
4. Aliphatic or aromatic amide
5. Ester-acid mixture
6. Percentage of keto-enol equilibrium
7. Equilibrium constant for ferric ion – salicylic acid complex (green method)
8. Extraction and analysis of coconut oil
9. Recinoleic acid and azelic acid from castor oil
10. Caffeine from tea leaves
11. Nicotine from tobacco leaves
12. Casein and lactose from milk
13. Green Soap: Extraction and saponification of avocado oil (green method)
14. Column chromatography: Separation of mixture of o and p-nitro anilines

References:
1. Brian S. Furniss, Antony J. Hannaford, Peter W. G. Smith and Austin R. Tatchell, Vogel's text book of Practical Organic Chemistry, 5th Edn. (8th impression), Pearson Education, New Delhi, 2011.
2. V. K. Ahluwalia and Renu Aggarwal, Comprehensive Practical Organic Chemistry: Quantitative Analysis, Universities Press (India) Pvt. Ltd., Hyderabad, 2013.
3. S. Warren, P. Wyatt, Organic Synthesis: The Disconnection Approach, John Wiley & Sons, New York, 2008
4. J. Clayden, Organic Chemistry, Oxford University Press, 2000
5. V.K. Ahluwalia and R.K. Parashar, Organic Reaction Mechanisms, 2nd Edn., Narosa publishing house, New Delhi, 2009
6. R. Bruckner, Advanced Organic Chemistry- Reaction Mechanisms, Academic press, San Diego, 2005
7. Jag Mohan, Organic Analytical Chemistry: Theory and Practice, Narosa publishing house Pvt. Ltd., New Delhi, 2006

CHM 6153: Multistep Organic Synthesis
[0-0-4-2]

Course Objectives:
At the end of the course students will be able to

- Perform multistep synthesis
- Choose the appropriate solvents for recrystallization

Pre-requisites:
B.Sc. Chemistry background

List of experiments
(Any ten experiments to be performed)
1. 2,4-Dinitrophenylhydrazine from chlorobenzene.
2. p-Aminoazobenzene from aniline.
3. 2,5-Dihydroxy acetophenone from hydroquinone.
4. Tribromobenzene from aniline.
5. Benzanilide from benzophenone.
6. Benzylic acid from benzoin.
7. Anthranilic acid from phthalic anhydride.
8. p-bromoaniline from acetanilide.
9. Methyl orange from aniline.
10. M-nitroaniline from nitrobenzene.
11. P-Chlorotolune from p-toluidine.
12. 2-Carbethoxycyclopentanone from adipic acid.
13. Aspirin (green method)

References:
1. A.I. Vogel, A Text Book of Practical Organic Chemistry, 5th Edn., Pearson, 2005
2. F.G. Mann, B.C. Saunders, Practical Organic Chemistry, 4th Edn., Pearson, 2009
3. R.K. Bansal, Laboratory Manual of Organic Chemistry, 5th Edn, New Age Int., 2008

Applied Chemistry Specialization

CHM 6161: Principles and Practice of Analytical Chemistry
[4-0-0-4]

Course Objectives:
At the end of the course students will be able to

- Explain the basics of analytical chemistry
- Identify a reagent or method for decomposition and dissolution reactions
- Describe separation and electro-analytical technique Apply organometallic

Pre-requisites:
B.Sc. chemistry background

Syllabus

Introduction:

Review of fundamental concepts of analytical chemistry. Statistical treatment, application of statistics to data treatment and evaluation, Hypothesis testing using statistical analysis, Using spread sheets for plotting calibration curves, Quality in analytical Chemistry, The basis and procedure of sampling, sampling statistics, sampling and physical state. 08

Decomposition and dissolution:

Reagents for decomposition and dissolution like HCl, H_2SO_4, HNO_3, $HClO_4$, microwave decompositions, combustion methods. 04

Elimination of interference from samples:

Separation by precipitation, electrolytic precipitation, extraction and ion exchange. Separation techniques based on phase equilibria: Principles of analytical separation, Craig concept of counter current distribution, process optimization, retention analysis, process optimization, Distillation: Fractional and molecular distillation. Separation technique based on rate process: dialysis, electrodialysis, electro-osmosis, reverse osmosis, electrophoresis and ultracentrifugation. 12

Electro-analytical techniques:

Brief review of conductometric and potentiometric titrations, High frequency titrations, Ion selective electrodes in potentiometry, Polarography and voltammetry, Cyclic voltammetry, Coulometry, Chronopotentiometry, Stripping analysis, Amperometric titrations, chronoamperometry 14

Environmental Analytical chemistry:

Introduction, analysis of atmospheric samples, analysis of water - Definition & estimation of Turbidity, pH, Acidity, Alkalinity, Hardness, Chlorides, DO, BOD, COD, Nitrogen, Solids, Fluorides, Sulphate, TOC, soil analysis, Thermal Methods in Environmental Analysis, Chromatography methods in Environmental Analysis. 10

References:

1. F.W. Fifield, D. Kealey, Principles and Practice of Analytical Chemistry, Blackwell Science, 2000

2. G.D. Christian, Analytical Chemistry, 4th Edn., John Wiely, 1986

3. S.M Kopker, Basic concepts of Analytical Chemistry, 2nd Edn., New age Int. Publications, New Delhi, 2002

4. D.A. Skoog, F. J. Holler, T. A. Nieman, Principles of Instrumental Analysis, 5th Edition, Saunders College Publishing, Chicago, 1998.

5. F. W. Fifield, P. J. Haines, Environmental Analytical Chemistry, 2nd Edn, Blackwell Science, London, UK, 2000.

CHM 6162: Analytical Chemistry Practical
[0-0-4-2]

Course Objectives:
At the end of the course students will be able to

- Illustrate the theoretical principles and major applications of electroanalytical techniques
- Demonstrate the theoretical principles and typical applications of chromatographic techniques
- Evaluate the accuracy and precision of experimental data and to demonstrate the application of statistical methods to refine the evaluation.
- Correlate spectra with structure of compound and Interpret the spectral data
- Prepare and characterize the polymer
- Study the factors affecting the rate of the reaction

Pre-requisites:
B.Sc. Chemistry background

(Any ten experiments to be performed)
List of experiments

1. Spectroscopic investigation of partition coefficient of iodine between H_2O and $CHCl_3$.
2. Verification of Beer's law
    a. Cu^{2+} - NH_3 system
    b. Fe^{3+} - KCNS system
3. Determination of composition and stability constant of metal complexes by (Fe^{3+} and salysilic acid, Ni (II) and 1,10 phenanthroline)
4. Determination of pKa values of maleic acid/malonic and phosphoric acid by potentiometric titration with sodium hydroxide using glass electrode.
5. Preparation of Polymethylmethacrylate by suspension polymerization, polystyrene/ Polyacrylamide by solution polymerisation method
6. Preparation of 6-10 Nylon by interfacial polymerization and its characterization by m.p, inherent viscosity and IR studies.
7. Ion-exchange chromatography: Separation and determination of Mg^{2+} / $Zn^{2+,}$ $Zn^{2+/}Cd^{2+}$; Cl^- /Br^-.
8. Separation of cations using column and paper chromatography
9. Determination of (a) COD and (b) DO in given sample of water.

10. To study the corrosion behavior of the given metal (a) without (b) with the addition of inhibitor by weight loss method./ Tafel method
11. Prediction of the structure of unknown simple organic compound based on the given FTIR, UV-Visible, 1H and 13C NMR spectra. (About 50 compounds have to be practiced).
12. Reaction between potassium persulfate and potassium iodide (including the study of effect of dielectric constant and catalysis by Ag^{+}/ Fe^{2+} / Cu^{2+} ions)
13. Error analysis and Statistical analysis of experimental data

References:

8. A.I. Vogel, A Text Book of Practial Organic Chemistry, 4th Edn. ELBS, 1992
9. F.J. Weicher, E. Robert, Standard methods of Chemical analysis, Krieger Publishing Co, 6th Edn, 1998
10. A.I. Vogel, A Text Book of Practial InOrganic Chemistry, 4th Edn. ELBS, 1992

CHM 6153: Applied Organic Chemistry Practical
[0-0-4-2]

Course Objectives:
At the end of the course students will be able to

- Quantify the percentage of organic compounds in a given sample
- Develop the skill in extracting the ingredients from the plant source
- Carryout organic reactions, work-up and recrystallization

Pre-requisites:
B.Sc. Chemistry background

List of experiments
(Any ten experiments to be performed)
1. Estimation of Glycine
2. Analysis of paracetamol
3. Estimation of aniline or acetone
4. Estimation of glucose
5. Analysis of amide-acid mixture
6. Lycopene from tomato
7. Extraction and analysis of groundnut oil
8. Piperine from pepper
9. Synthesis of acetylamino cinnamic acid from glycine
10. Preparation of ethyl resorcinol from resorcinol
11. Anthranilic acid from phthalic anhydride
12. Benzopinacolone from benzophenone

References:
1. A.I. Vogel, A Text Book of Practical Organic Chemistry, 5th Edn. Pearson, 2003
2. F.G. Mann, B.C. Saunders, Practical Organic Chemistry, 4th Edn. Pearson, 2009.
3. R. K. Bansal, Laboratory Manual of Organic Chemistry, 5th Edn, New age Int, 2008

4th Semester

CHM 60xx: Elective II
[3-0-0-3]

The department will offer three papers from the basket of electives. The students has to give their preferences. If the number of students opting for a particular elective is less than 5, such students' second preference will be considered.

CHM 60xx: Elective III
[3-0-0-3]

The department will offer three papers from the basket of electives. The students has to give their preferences. If the number of students opting for a particular elective is less than 5, such students' second preference will be considered.

CHM 6201: Project Work
The project work has to be carried out in the institution. The duration of the project work shall be of 16 weeks. The evaluation will be through mid-term presentation and end-semester presentation. The oral presentation and project report will be evaluated by the department committee for project evaluation.

Organic Chemistry Specialization

CHM 6251: Advanced Organic Chemistry II
[4-0-0-4]

Course Objectives:
At the end of the course students will be able to

- Describe the syntheses and reactions of non-aromatic heterocyclic compounds, heterocyclic compounds having one or more hetero atoms
- Demonstrate an understanding of different types of natural products such as alkaloids, terpenoids, carotenoids and steroids
- Describe the examples and chemical properties of natural products
- Explain the synthesis of some natural products and their structure-activity relationships.

Pre-requisites:
CHM 6102

Syllabus

Non aromatic Heterocycles:

Nomenclature, Strain- bond angle and torsional strains, interactions and conformational aspects of nonaromatic heterocycles. Synthesis, reactivity and importance of the 3, and 4 membered ring systems. 06

Aromatic Heterocycles:

General chemical behavior of aromatic heterocycles, criteria of aromaticity Heteroaromatic reactivity and tautomerism in aromatic heterocycles. Preparation, properties and applications of pyrrole, furan, thiophene, Pyrazole, Imidazole, Oxazole, Thiazole, benzopyrroles, bezofurans and benzothiophenes. benzopyrazole, benzimidazole, benzoxazole and benzthiazole, 12

Six membered ring system:

Synthesis and reactions of pyridine, pyran, quinoline, isoquinoline, acridine and phenanthridine, 2-pyrones, 4-pyrones, benzopyran, benzo-2-pyrones and benzo-4-pyrone, Preparation of pyridazine, pyrimidine, pyrazine, 06

Alkaloids and Terpenoids:

Classification, Isolation, Methods of structural determination of alkaloids. Steriochemistry, synthesis of Adrenaline, Ephedrine, Quinine, Applications, Structure, classification and isolation of mono - and sesqui - terpenoids, isoprene rules, methods of determining structure of terpenoids, α-pinene, camphor, borneol, isoborneol, nerolidol, zingeberene. 12

Carotenoids and Steroids:

Geometrical isomerism of carotenes, Structure and synthesis of β-carotene, Structure and synthesis of anthocyanins, flavones, isoflavones. Introduction and Nomenclature of steroids, Blanc's rule, Barbier-Wieland degradation, Oppenauer oxidation, Diel's hydrocarbon, Chemistry of Cholesterol, Ergosterol, bile acids. oestrone, oesterdiol, oestriol, progesterone, androsterone, aldosterone, testosterone, cortisone, and cortisol. 12

Reference:

1. Raj K. Bansal, *Heterocyclic chemistry,* 3rd Edn., New Age International (P) Ltd., 1999
2. J.A. Joule & K.Mills, *Heterocyclic Chemistry,* 4th Edn., Blackwell publishing, 2000
3. T. Eicher and S. Hauptmann, *The Chemistry of Heterocycles*.2nd Edn.,Wiley-VCH, 2003
4. Gurdeep R Chatwal, Organic Chemistry of Natural Products Vol 1 and 2, Himalaya Publishing House, 2011
5. O. P. Agarwal, Organic Chemistry Natural Products Vol 1 and 2, Krishna Prakashan Media (P) Ltd, 2018

Applied Chemistry Specialization
CHM 6261: Nuclear and Radiation Chemistry
[4-0-0-4]

Course Objectives:
At the end of the course students will be able to

- describe the nuclear structure, properties and decay processes
- explain the various nuclear reactions and different types of radiation detection
- discuss the radio isotopes and their applications in various fields
- explain the synthesis of transuranium elements and health & safety aspects of radiation..

Pre-requisites:
B.Sc. chemistry background

Syllabus

Introduction to Nuclear Chemistry:

The Nucleus and Nuclear structure: Nomenclature, properties of nucleus – Nuclear masses, binding energy per nucleon, separation energy systematics, semiemperical mass equation, nuclear sizes and shapes, quantum mechanical properties – nuclear anguar momentum, electric and magnetic moments, magnetic dipole moment, electric quadrupole moment. Nuclear structure: Liquid drop model, shell model, collective model, Nilsson model and Fermi gas model. Decay systematics: alpha decay, beta decay and gamma decay. alpha decay – energetics, theory, hindrance factors, heavy particle and proton radioactivity, beta decay – neutrino hypothesis, rate constant, electron capture decay, parity non conservation, beta delayed radio activities, gamma decay – energetics, classification of decay types, electromagnetic transition rates, internal conversion, angular correlations, Auger electrons, nuclear isomerism, isomeric transitions. 14

Nuclear reactions:

Energetics of nuclear reactions, reaction types and mechanisms, nuclear reaction cross sections, direct reactions, compound nuclear reactions, photonuclear reactions, Heavy ion reactions, fusion reactions, high energy nuclear reactions, fragmentation reactions, reactions induced by radioactive projectiles. 5

Introduction to Radiation Chemistry:

Radioactive decay modes of natural and artificial nuclides, Determination of half-life, decay and growth kinetics, Conditions of equilibrium theories of α, β, and γ emissions. 3

Radio isotopes:

Definition of curie and related calculations. Production of radioisotopes and labelled compounds by bombardment. Radiochemical separation techniques- carriers, solvent extraction and ion-exchange methods. Physico chemical and analytical applications of radioisotopes- isotope dilution method, activation analysis, radiometric titrations, 14C dating. Medical, agricultural and industrial applications of isotopes. Radiation sources, units (LET, Rad, Roentgen and G-value), radiation dose and radiation chemical yield. Chemical Dosimetry-Fricke and ceric sulphate

dosimeters. Radiation chemistry of water. A brief introduction to radiolysis of gases, liquids and solids. Techniques for study of transient species- Pulse radiolysis. Industrial applications of radiation chemistry (radiation polymerization, food irradiation and radiation synthesis). 14

Radiation Detectors:

Principles of counting techniques such as G.M. counter, proportional, ionization and scintillation (solid and liquid) counters. Cloud chamber, nuclear track detectors, neutron detectors 4

Transuranium elements and Nuclear Reactor Chemistry:

Synthesis of transuranic elements such as Neptunium, Plutonium, Curium, Berkelium, Einsteinium, Mendelevium, Nobelium, Lawrencium and elements with atomic numbers 104 to 109, Types of nuclear power reactors, basic features and components of nuclear power reactors. An introduction to breeder reactor. 4

Health and Safety Aspects:

Biological effects of radiation, Hazards in radiochemical work. Radiation protection, permissible exposure doses. Radioactive waste management. 4

Reference:

1. Walter D. Loveland, David J. Morrissey and Glenn T. Seaborg, Modern Nuclear Chemistry, 2nd Ed., Hoboken, NJ: John Wiley & Sons, Inc., (2017)
2. C. A. Bertulani and P. Danielewicz, Introduction to Nuclear Reactions, CRC Press (2004)
3. Choppin, Liljenzin and Rydberg, Radiochemistry and Nuclear Chemistry, 3rd ed., Butterworth=Heinemann press, (2002)
4. Robert E. Masterson, Nuclear Engineering Fundamentals: A practical perspective, 1st ed. CRC press, (2017)
5. Friedlander, Kennedy Macias and Miller, Nuclear and Radiation Chemistry, Wiely (1985)
6. H. J. Amikar, Essentials of Nuclear Chemistry, Wiley Eastern (1987)
7. Spinks and Woods, Radiation Chemistry: Principles and Applications, VCH, Weinheim (1999)

Electives

CHM 6001: Materials Chemistry
[3-0-0-3]

Course Objectives:
At the end of the course students will be able to

- Understand the fundamental principles of material science
- Define liquid crystal phases and give specific examples and properties of various types
- Discuss the concepts and applications of nanomaterials and thin films
- Explain the functional needs and designs to various kinds of material production

Pre-requisites:
B.Sc. Chemistry background

Syllabus

Introduction:
Fundamental principles, Classification of materials- Solid materials. Advanced materials, Nano-materials, Review of bonding in solids 06

Liquid Crystals:
Introduction to liquid crystals, Thermotropic and lyotropic liquid crystals, Positional order, Nematic, Chiral nematic, Twisted nematic and smectic mesophases, Clearing temperature and optical properties, Organic LEDs, Organic semiconductors. 06

Nanomaterials:
Fundamentals of nanomaterials, Technological advantages of nanomaterials, Synthesis of nanomaterials: Top-down (Nanolithography, CVD), Bottom-up (Sol-get processing, chemical synthesis). Wet Deposition techniques, Self-assembly (Supramolecular approach). Characterization: TEM, SEM and SPM technique, Fluorescence Microscopy and Imaging. Carbon nanotubes, wires, and quantum dots. Applications in solar energy conversion and catalysis, applications in polymers with a special architecture, Applications in photonics, plasmonics, chemical and biosensors, medicine and biotechnology. 14

Thin films:
Fabrication of thin films, Physical Vapor deposition (PVD), Advantages of PVD, Disadvantages of PVD, Applications of PVD, Chemical Vapor Deposition (CVD), Advantages of CVD, Drawbacks of CVD, Applications of CVD, Comparison between CVD and CVD. 04

Materials of engineering applications:
Metals and alloys, Cement, Ceramics, Silicon and the chip, Composite materials, smart materials, Polymer composite materials, Refractories and abrasives and biomaterials.

06

References

1 Bradley D. Fahlman, *Materials Chemistry*, 3rd ed., Springer, Dordrecht, 2018.
2 *Molecular Soft-Interface Science: Principles, Molecular design, Characterization and Application*; Mizuo Maeda, Atsushi Takahara, Hiromi Kitano, Tetsuji Yamaoka and Yoshiko Miura (ed.), Springer, Tokyo, 2019.
3 S. M. Lindsay, *Introduction to Nanoscience*, Oxford University Press Inc., New York, 2010.
4 M.A. Shah, T. Ahmed, *Nano Science and Nano Technology*, Narosa Publishing House, New Delhi, 2010
5 Lev M. Blinov, Structure and Properties of Liquid Crystals, Springer, Dordrecht, 2011.
6 W.D. Callister,Jr, *Callister's Materials Science and Engineering*, John Wiley and Sons. 2007

CHM 6002: Industrial process and Industrial management
[3-0-0-3]

Course Objectives:
At the end of the course students will be able to

- Develop skills in supervision of any activity
- Equip with skills necessary for effective communication
- Enable to use the available resources to achieve the desired goal in a more efficient and effective way
- Develop skills in present-day management methods in the workplace, using many software and hardware tools

Pre-requisites:
B.Sc. Chemistry background

Syllabus

Industrial Process and Economics

Basic concepts of Industrial economics.
Methods employed for the estimation of capital investment, capital formation – Fixed capital and working capital. Economic Flow Chart – External Sources and Internal Sources, Financial Requirement – Comparative Evaluation. Elements of cost accounting – Direct cost, indirect cost and behavior of cost. Factors involved in project cost estimation. Interest and investment cost. Time value of money equivalence. Break-even analysis: Assumptions, break even chart, optimum batch sizes, production scheduling. Depreciation, Methods of determining depreciation, taxes. Profitability criteria, economics of selecting alternatives. Variation of cost with capacity, Planning: Advantages, objectives – Management Objectives. Budget. 16

Industrial Management

Introduction, Preliminary project report – Aim, Purpose and techniques adopted during preparation of the project report. Location of Industry – Factors, Criteria, Determination of lower cost site. Scientific functions of management – Traditional management, drawbacks, aim and objectives of scientific management. Functions of management – management functions and responsibilities – decision making. Marketing – Definition, marketing concept, sales forecast, market segmentation. Advertising – Definition, objectives and aims, functions of advertising, essentials of good advertising. Material Management - Significance and purchasing method. Decision making, organizing, directing and control. Departmentation principles, span of control forms of organization structure - organization charts. Human resources management- Recruitment, Training. Industrial safety. Employee's welfare selection, Incentives and motivation, safety. Industrial safety and welfare. Centralization - Reasons, advantages and disadvantages. Decentralization - Advantages and disadvantages. 20

References

1. T.R. Jain, O.P. Khanna, *Process Economics,* Global publication Pvt. Ltd., 2010.
2. C.R. Thomas, S.C. Maurice, S. Sarkar. *Managerical Economics,* 9th Edn., Tata McGraw Hill education Pvt. Ltd., New Delhi, 2010.
3. Robert A. Smiley, Harold L. Jackson, Chemistry and the Chemical Industry: A Practical Guide for Non-Chemists, CRC Press CRC Press, 2002.
4. R. D. Agrawal, Organization and management, McGraw Hill Education; 1 edition 2017.
5. M.S. Mahajan, Industrial Management, Dhanpat Rai & Co, 2013.

CHM 6003: Chemistry of Dyes and Pesticides

[3-0-0-3]

Course Objectives:

At the end of the course students will be able to

- understand the basics of dyestuff industry in terms of raw materials utilized
- understand basic benzene and naphthalene chemistry.
- analyze the various methods for synthesis of different intermediates used in dyes
- know the various technology and safety aspects for reactions.
- understand the basics of dyestuff industry in terms of raw materials utilized

Pre-requisites:

B.Sc. Chemistry background

Syllabus

Dyes

Introduction, modern theories of colour and chemical constitution. A general study of the following: Direct azo dyes (congo red, rosanthrene O, procion dyes), acid azo dyes (ponceau 2R, Naphthol blue black 6B), basic azo dyes (chrysoidin G, bismark brown), developed dyes, mordent dyes, vat dyes, disperse dyes, fibre reactive dyes, sulphur dyes and solvent dyes. Fluoroscent brightening agents (tinopal B.V), cyanine dyes

(classification, application in photography, quinoline blue and sensitol), chemistry of colour developer, and instant colour processes. Synthesis and applications of malachite green, rhodamine-B, phenolphthalein and methyl orange. Triphenylmethane dyes: crystal violet, pararosaniline, aurin, chromeviolet. Application of dyes: i. photography, ii. Biological studies. **19**

Pesticides

Introduction, classification, mode of action and synthesis of chlorinated pesticides (DDT, chlordane, heptachlor and hexachlorocyclohexane), Naturally occurring pesticides pyrethroids-natural pyrethrins-isolation and structures, synthetic pyrethroids, allethrin, cypermethrin, phenvalerate. Organophosphorous pesticides: Malathion, parathion, DDVP, diazenon. Carbamate pesticides: Sevin, carbofluron, aldicab, beygon. Insect Pheromones: Introduction, classification, use in insect pest control. Synthesis of disparlure, faranol, grandisol, brevicomin and bomykol. Fungicides: Introduction, Inorganic & organic fungicides, Systemic fungicides-types & examples. Herbicides: Introduction, study of sulfonyl ureas, heterocyclic sulfonamides, heterocyclicamines,dihydropyrano[2,3-b]pyridylimidazolinones, pyrrolopyridyl-imidazolinones, 1,2,4-triazine-3,5-diones, hydroxyoxazolidinones & hydroxypyrrolidinones, pyridine herbicides & 1,3,4-oxadiazoles. Mechanism of action and toxicities of insecticides, fungicides and herbicides. **17**

References

1. Padma Vankar, *Natural Dyes for Textiles* 1st Edition, Woodhead Publishing, 2017
2. O.D. Tyagi, M. Yadav, A text book of Synthetic Dyes, 2002
3. H. Panda, *Modern Technology of Textile Dyes & Pigments* (2nd Revised Edition), 2016
4. NIIR Board of Consultants & Engineers, *The Complete book on Natural Dyes & Pigments,* Asia Pacific Business Press Inc. 2005
5. Simon J. Yu, The Toxicology and Biochemistry of Insecticides, 2nd Edition, CRC Press, 2014

CHM 6004: Chemistry of Petrochemicals

[3-0-0-3]

Course Objectives:

At the end of the course students will be able to

- Understand various petroleum refinery processes
- Know the manufacturing methods of various petrochemicals
- Describe various catalysts used in petroleum industry and the preparation of zeolites
- Discuss the classes of lubricants, properties and their determination

Pre-requisites:

B.Sc. Chemistry background

Syllabus

Petroleum and Refining:

Origin and formation of Petroleum, Reserves and deposits of world and Indian Petroleum Industry, Composition of crude Petroleum and natural gas, Characterization of crude oil, pre-treatment of crude, removal of moisture, salts etc. Refining and different types of petroleum products and their applications. Overview of Petroleum Refinery - Petroleum Refinery types, Processes and operations, Petroleum Refinery flow schemes, Definitions of Refining terms. Economic, health and environmental issues related to petroleum refining. Distillation of crude oil, Separation and constituents of natural gas, atmospheric distillation, vacuum and pressure distillation, Fractional Distillation (Principle and process), composition of different distillates, types of hydrocarbon groups present in petroleum and their structures, sulfur, nitrogen, oxygen and organo-metallic compounds in petroleum, pour point depressants, drag reducers, viscosity reducers, ignition point, flash point, octane number, Process and mechanism – cracking (Thermal and catalytic cracking), Hydrocracking, Isomerization, Reforming, Alkylation, Manufacture of synthetic petrol - Bergius and Fischer Tropsh processes. 12

Manufacture of petrochemicals:

Methane, ethylene, acetylene, propylene, C–4 hydrocarbons, higher olefins. Preparation of the following from methane – methanol, carbon black, hydrogen cyanide, chlorinated methanes and carbon disulphide. Preparation of the following from ethylene – Ethyl chloride, ethanol, ethylene oxide, ethylene glycol, acetaldehyde, acetic acid, styrene, vinyl acetate, ethanolamines, vinyl chloride and acrylonitrile. Manufacture of the following from propylene - Isopropanol, cumene, glycerine and acrylonitrile. Manufacture of the following from acetylene - vinyl chloride, chloroprene, acrylonitrile and acetaldehyde. Manufacture of the following from C–4 hydrocarbons: Butadiene, isobutene and isobutene. Manufacture of linear alkyl benzenes and their sulphonates, phenol, Toluene and its derivatives Xylene, butanediols, oligomers. Possible green methods / advanced methods of synthesis of above petrochemicals 12

Catalysts used in petroleum industries:

Structure, selectivity and applications, classification, acidity and basicity in Zeolites, Zeolite synthesis reactions, unit cell structure, cation exchange, dealumination and isomorphus substitution principles, Applications of Zeolites in catalysis and in separation processes- a few case studies 06

Lubricants:

Classification of lubricants, lubricating oils (conducting and non-conducting), solid and semisolid lubricants, synthetic lubricants. Properties of lubricants (viscosity index, cloud point, pore point) and their determination. 06

References:

1. Saikat Maitra, O. P. Gupta, *Elements of Petrochemical Engineering*, Khanna Book Publishing, New Delhi, 2018.
2. B.K.B. Rao, *Modern Petroleum Refining Processes*, 4th Edn., Oxford and IBH Publishing Co. Pvt. Ltd., New Delhi, 2005

3. Sami Matar and Lewis F. Hatch., *Chemistry of Petrochemical Processes*, 2nd ed., Gulf Professional publishing, Saudi Arabia, 2001.
4. Ram Prasad, *Petroleum refining technology*, 1st Ed., Khanna book publishing, New Delhi, 2002.
5. G.N. Sarkar, *Advanced Petroleum Refining*, 1st Edn., Khanna Publishers, Delhi, 1998
6. S. Maiti, *Introduction to Petrochemicals,* 2nd ed. Oxford and IBH Publishing Co. Pvt. Ltd., New Delhi, 2002

CHM 6005: Applied Electrochemistry and Industrial Catalysis
[3-0-0-3]

Course Objectives:
At the end of the course students will be able to

- Explain certain key concepts in corrosion
- Understand application of electrochemistry and catalyst in industrial scale

Pre-requisites:
B.Sc. Chemistry background

Syllabus

Corrosion and its control:

Corrosion basics: Importance of corrosion, Corrosion classification : dry and wet corrosion; electrochemical theory, Brief discussion on eight forms of corrosion, Factor affecting corrosion Kinetics of corrosion: Butler- Volmer equation, mixed electrode potential theory, Evans diagram, Thermodynamics of corrosion: free energy concept and Pourbaix diagram, Corrosion rate: Units for expressing corrosion rate, Corrosion rate measurement techniques: Weight loss method, potentiodynamic polarization method, electro chemical impedance method. Need of corrosion control, Corrosion control techniques with special reference to corrosion inhibition. 14

Industrial electrochemistry:

Electro synthesis: fundamental principles; comparison between chemical and electrochemical synthesis; Green chemistry and electro-synthesis; Experimental set up for electro-synthesis, Electron transfer, Mass transfer, adsorption, electro-catalysis. Kolbe's synthesis, electro oxidation of hydrocarbons, electro reduction of halogen, nitro, carbonyl compounds, Reductive and oxidative coupling reactions, Electro inorganic synthesis -, chlorate, ozone and electrofluorination. Advantageous, limitations and possible solutions for electro-synthesis 10

Industrial Catalysis

Overview of catalysis, Preparation of catalyst and their behavior Role of supports, preparation and structures of supports like silica, alumina, zeolites, and carbon. Deactivation process: sintering, poisoning and catalyst fouling, Performance criteria of catalyst: activity, selectivity, temperature response, catalyst life.

Industrial applications of catalysts in oxidative de-hydrogenation, oxidative organic transformations, partial oxidation reactions, alkylation of amines, Production of petrochemicals, Catalytic reforming and refining, catalytic cracking, hydro-treatment, steam reforming, hydrocarbon from synthesis gas, Fischer-Tropsch process, Mobil process for conversion of methanol to gasoline, Catalysis for polymerization, Brief account of bio-catalysis. 12

References:

1. D.R. Crow, Principles and applications of electrochemistry, 6th Edn. Chapman and Hall Publications, 2000
2. E. Mc Cafferty, *Introduction to Corrosion Science*, Springer, 2013
3. R.N. Shereves, *Chemical Process Industries, 4th Edn., McGraw Hill, New York 2012*
4. H. Lund, O. Hammerich, *Organic Electrochemistry* 4th Edn., Marcel Dekker, New York, 2001
5. B. Vishwanathan, *Catalysis Principles and Applications*, Narosa Publications, 2011

CHM 6006: Green Chemistry
[3-0-0-3]

Course Objectives:
At the end of the course students will be able to

- Define green chemistry and identify the challenges of green chemistry
- Explain the principles of green chemistry and recognize the green criteria in the practice of chemistry
- Identify reagents solvents and processes that could be replaced by green alternatives

Pre-requisites:
B.Sc. Chemistry background

Syllabus

Introduction:

Definition of green chemistry, Green chemistry tools - Alternate starting materials, reagents, solvents, products and catalysts, twelve principles, Evaluating the effects of chemistry, evaluating starting materials, reaction types, methods to design safer chemicals. Green chemistry matrices - Atom economy, eco-factor, Effective mass yield, Reaction mass efficiency and Carbon efficiency, Examples of green chemistry – starting materials, reactions, reagents, solvents and chemical products. Chemicals from biomass, Case studies to illustrate the use of alternative feedstock, reagents & reaction media. Green synthesis of nanomaterials, life cycle considerations, Product and process design for sustainability, CLP and REACH. 10

Catalysis and Green Chemistry:

Importance of selective catalysts in sustainable development, Selectivity in catalysis - chemoselectivity, regioselectivity, enantioselectivity, shape-selectivity, Catalysts for clean technology including life cycle assessment issues, Heterogenisation of homogeneous

catalysts - its role in waste minimization, Adsorbates and adsorbents, Preparation of supported reagents and Applications. Catalysis in various chemical industries - bulk chemicals: alkylation of aromatic compounds, selective oxidation reactions, manufacture of adipic acid, phenol, and caprolactum, Fine chemicals: hydroxylation of phenol, synthesis of vanillin, production of citral, aziridine and lazabemide. 06

Cleaner Production:

Examples of cleaner production, Design of environmentally benign processes, Use of microwaves, ultraviolet and infrared radiations for clean syntheses, Commercially developed insecticides based on natural products, Ecofriendly biopesticides, Use of enzymes in oxidation, reduction and hydrolysis reactions, Electrochemical synthesis - adiponitrile and sebasic acid, Industrial case studies – manufacture of polymer, pesticide, food & flavor, dye, paper & pulp, and pharmaceutics. 06

Alternate Reaction Media:

Overview of solvent properties, Solvents - reactions in multiphase solvent systems, Green solvents, Fluorous biphasic systems, ionic liquids, crown ethers, supercritical fluids – CO_2, Synthetic applications of Fluorous biphasic systems, ionic liquids, supercritical fluids, Crown ethers and quarternary ammonium salts, Water as solvent: Diels-alder, aldol condensation, selective oxidation and reduction reactions, Phase transfer catalysis in syntheses – examples. 07

Control of Environmental Impact:

Environmental impact of chemical substances & fuels, Environmentally benign reactions, Environmental management system, Control & monitoring of chemical processes, products & waste, Waste minimization techniques, Photochemical degradation of waste treatment, Phosphate removal, Reduction in volatile organic compounds in the atmosphere, Water purification, Water disinfection & trihalomethanes. 07

References:

1. P.T. Anastas, J.C. Warner, *Green Chemistry*: *Theory and Practice*, Oxford Univ. Press, Oxford, 2008
2. A.S. Matlack, *Introduction to Green Chemistry*, Marcel Dekker, New York, 2001
3. P.T. Anastas, R. H. Crabtree, *Hand Book of Green Chemistry and Catalysis*, Wiley, New York, 2009
4. M. Lancaster, *Green Chemistry – An Introductory Text,* RSC, Cambridge, 2002
5. R. Sanghi, M.M. Shrivastava, *Chemistry for Green Enviornment*, Narosa Publishing House, New Delhi, 2007
6. V. K. Ahluwalia, Green Chemistry – A Text book, Narosa Publishing House, New Delhi, 2007
7. Marteel-Parrish Anne E-Abraham Martin A - Green Chemistry and Enginnering- A Pathway to Sustainability, Wiley 2009

CHM 6007: Organometallic Cluster Chemistry
[3-0-0-3]

Course Objectives:
At the end of the course students will be able to

- Explain certain key concepts in organometallic cluster chemistry (e.g.PSEPT, bonding)
- Use these concepts in cluster chemistry problem solving
- Describe the chemistry of transition metal clusters and the industrial applications

Pre-requisites:
B.Sc. Chemistry background

Syllabus

Chemical Background & Cluster Classification

Overview of organometallic chemistry, Metal-metal bonds and metal atom clusters, Factors favoring the formation of metal-metal bonds, Clusters as a bridge between molecules and solids, Opportunities offered by clusters, Types of clusters with examples: homonuclear and heteronuclear, low and high valence, cyclic and acyclic, and ligated and naked, etc. 07

Synthetic Strategies & Methods of Characterization

Commonly employed methods- Pyrolytic decarbonylation, Redox condensation, Metal exchange reactions, Recent alternative approaches-Bridge-assisted reactions, Addition across multiple bonds, Addition of unsaturated moieties, Infrared spectroscopy, NMR spectroscopy, Mass spectrometry, Electronic absorption spectroscopy, X-ray diffraction and other methods, Structures of Metal Clusters -Trinuclear clusters,Tetranuclear clusters, Pentanuclear clusters, Hexanuclear clusters, High nuclearity clusters, Structural patterns. 08

Bonding and Electronic Structure Considerations

Bonding modes of common ligands on clusters (H, CO, S, C_2R_2, Cl), Bonding theories as applied to clusters, The 18-electron rule, Polyhedral skeletal electron-pair theory, Topological electron counting, Lauher's cluster model, The isolobal analogy in metal clusters. 06

Basic Metal Cluster Reactions

Electron transfer reactions, Addition, elimination and substitution reactions, Cluster expansion and degradation reactions, Cluster framework rearrangements, Cluster protonation and deprotonation. 08

Industrial Aspects of Cluster Chemistry

Homogeneous cluster catalysis, Modeling studies and heterogeneous catalysis, Activation of small molecules on clusters- Cluster-assisted ligand transformations, Application to organic synthesis, Isomerization and stereochemical nonrigidity, Other

Applications- Thin films by MOCVD using cluster precursors, Molecules to solids transformation, Optically active clusters, Biological models 07

References

1. Paul J. Dyson, J. Scott McIndoe, Transition metal carbonyl cluster chemistry, First Edition, CRC Press, 2000
2. Pierre Braunstein, Luis A. Oro, Paul R. Raithby, Metal Clusters in Chemistry, Wiley -VCH, Weinheim, 1999
3. Rosenberg, E; Laine, R, Concepts and models for characterizing homogeneous reactions catalyzed by transition metal cluster complexes. New York: Wiley-VCH, 1998
4. Jos de Jongh, L, Physical properties of metal cluster compounds. Model systems for nanosized metal particles. New York: Wiley-VCH, 1999

CHM 6008: Polymer Chemistry
[3-0-0-3]

Course Objectives:
At the end of the course students will be able to

- Describe the bonding in polymers, molecular weight and its distributions, geometrical structure of polymer molecules, structure-property relationships.
- Understand the mechanisms and techniques of polymerization.
- Illustrate the synthesis, properties, and applications of some important commercial polymers.
- Explain the reactions of polymer with specific groups. degradation types, biodegradation and management of plastics in environment.
- Understand the methods of polymer processing.

Pre-requisites:
B.Sc. Chemistry background

Syllabus

Introduction to Polymers:
Basic concepts, Molecular forces and Chemical bonding in polymers, Molecular weight and its distribution, Structure property relationship- Physical, mechanical and theological properties. Chemical and geometrical structure of polymer molecules 08

Polymerization – Mechanism and Techniques:
Addition, Condensation, Coordination, Copolymerization, Metathetical, Group-transfer polymerization, Polymerization techniques- bulk, solution, suspension, emulsion, poly-condensation, solid and gas phase polymerization. 08

Commercial polymers-synthesis, properties and applications:
Synthesis, properties, structural features and applications of some important commercial polymers, Engineering specialty polymers, Applications in separations, medicine, electronics-conducting polymers, biomedical. 08

Polymer reactions and degradation:
Reactions of various specific groups, cyclisation, crosslinking, modification of commercial polymers. Types of degradation – Thermal, oxidative, hydrolytic, mechanical, photo and ultrasonic. Management of plastics in environment- recycling, incineration, biodegradation. 06

Polymer processing
Elastomer processing, Molding-Injection, Blow, Rotational, Compression and Transfer, Thermoforming, Casting, Extrusion, Calendering, Coating, Reinforced plastics (composites) and laminates. 06

Reference:

1. F.W. Billmeyer, *Text book of Polymer science*, 3rd Edn., A Wiley- Interscience Publication, New York, 2005
2. V.R. Gowariker, *Polymer Science*, New Age International (P) Ltd., New Delhi, 2012
3. P. C. Hiemenz and T. P. Lodge, *Polymer Chemistry*, 2nd Edn., CRC Press, Taylor & Francis group, New York, 2007
4. W. S. Allen and P. N. Baker, S. C. Bhatia (Ed.), *Hand book of Plastic Technology-Plastic Processing Operations*, vol. 1, 1st Edn., CBS Publishers & Distributors, New Delhi, 2004
5. J.R. Fried, *Polymer Science and Technology*, Prentice Hall of India Pvt. Ltd., New Delhi, 1999

CHM 6009: Supra molecular chemistry
[3-0-0-3]

Course Objectives:
At the end of the course students will be able to
- Explain the concepts of supramolecular chemistry
- Describe supramolecular catalysis. devices and sensors

Pre-requisites:
B.Sc. Chemistry background

Syllabus
Crystal engineering
Concepts and Languages of supramolecular chemistry. Various types of non-covalent interactions. Hydrogen bonds, C-H…X interactions, Halogen bonds. π–π interactions, non–bonded interactions. Various types of molecular recognition.

Crystal engineering of Organic solids: Hydrogen bonded supramolecular patterns involving water / carboxyl / halide motifs. Concepts of different types of synthons based on non-covalent interactions. Principles of crystal engineering and non-covalent synthesis. Polymorphism and Pseudopolymorphism. Supramolecular isomorphism / polymorphism. Crystal engineering of pharmaceutical phases. 12

Crystal structure and receptors

Co-receptor Molecules and Multiple Recognition: Dinuclear and Ploynulclear Metal ion Cryptates. Linear recognition of molecular length by Ditopic Coreceptors. Heterotopic Co-receptors- Cyclophane Receptors, Amphiphillic Receptors, Large molecular cages. Multiple Recognition in Metalloreceptors. Supramolecular dynamics.

Supramolecular Reactivity and Catalysis

Catalysis by Reactive Macrocyclic Cation Receptor Molecules. Catalysis by Reactive Anion Receptor Molecules. Catalysis with Cyclophane Type Receptors. Supramolecular Metallocatalysis. Cocatalysis: Catalysis of Synthetic reactions. Biomolecular and Abiotic catalysis

Supramolecular Chemistry in solution: Cyclodextrin, Micelles, Dendrimmers, Gelators. Classification and typical reactions- Applications. 12

Supramolecular Devices and Sensors

Various types of supramolecular devices – an overview.

Supramolecular Photochemistry: Molecular and Supramolecular Photonic Devices – Light conversion and Energy Transfer Devices. Molecular and Supramolecular Electronic Devices – Electronic conducting Devices - Molecular wires, Modified and Switchable Molecular wires. Molecular and Supramolecular Ionic Devices – Tubular Mesophases, Molecular Protonics. Switching Devices: Photo switching and Electroswitching. Ion and molecule sensors. Role of supramolecular chemistry in the development of nanoscience and technology. 12

References:

1. A.R. West, Solid State Chemistry and its Applications, VCH, Wienheim, 2014.
2. E. R. T. Tiekink, J. Vittal, M. Zaworotko, Organic Crystal Engineering: Frontiers in Crystal Engineering, John Wiley & Sons, 2010
3. J.M. Lehn, *Transition metals in supramolecular chemistry*, John Wiley & sons, New York, 1999
4. J.W. Steed, D.R. Turner, K. J. Wallace, *Core Concepts in Supramolecular Chemistry and Nanochemistry*, John Wiley & Sons, New York, 2007
5. J.W. Steed, J. L. Atwood, *Supramolecular Chemistry*, John Wiley & Sons, New York, 2002

CHM 6010: Solid State Chemistry and Applications

[3-0-0-3]

Course Objectives:

At the end of the course students will be able to

- Define amorphous - crystalline solids, defects in solids
- Discuss the various preparative methods
- Describe the properties and application of solid-state materials

Pre-requisites:
B.Sc. Chemistry background

Syllabus

Introduction of Crystal Structure

Crystalline and amorphous solids; types of close packing- hcp and ccp, packing efficiency, radius ratios; polyhedral description of solids; Structure types – NaCl, ZnS, Na_2O, $CdCl_2$, Wurtzite, CdI_2, Rutile, Perovskite ABO_3, K_2NiF_4, Spinels.
Solid State Reactions: Vapor phase transport, preparation of thin films - electrochemical methods, chemical vapour deposition. 07

Preparative methods

Solid state reaction, chemical precursor method, co-precipitation, sol-gel, metathesis, self-propagating high temperature synthesis, ion exchange reactions, intercalation / deintercalation reactions, hydrothermal and template synthesis, high pressure synthesis.
Crystal growth – Czochralski Growth of Single Crystals, Bridgman & Stokbarger methods, zone melting, zone refining.
Defects in crystals: Point defects, Defect equations, vacancy concentration in a metal, Schottky defect concentration in an ionic crystal, Frenkel defect concentration, Dislocations, Plane defects or Grain Boundaries. 14

Introduction to the solid state

Amorphous solids - Crystalline solids. Oxide Ion Conductors, Fluoride, Silver, Copper ion, Lithium ion and Proton Conductors. Solid polymer Electrolytes. Application of Solid Electrolytes. Fuel cells: electrochemical power generator (hydrogen-oxygen cell, Solid state Galvanic cell). 08

Characterization

Magnetic properties: Introduction and classification of magnetic material (Dia, Para, ferro, antiferro, ferimagnetism).
Optical properties: Luminescene (Frank-condon principle, Laser and maser action, application of laser)
Dielectric properties, Piezo electric materials.
Superconductivity: Basics, discovery and high temperature materials. 07

Reference

1. D.K. Chakrabarty, *Solid State Chemistry*, New Age International Publishers, 2010
2. R.C. Ropp, *Solid State Chemistry*, Elsevier, 2008
3. A.R. West. *Solid State Chemistry and its Applications*, John Wiley 2007
4. P.J. Gellings, H.J.M. Bouwmeester, *Solid State Electrochemistry*, CRC press, 1997

CHM 6011: Chemical Process Industries
[3-0-0-3]

Course Objectives:
At the end of the course students will be able to

- Read and interpret basic process industry drawings.
- Identify and describe basic equipment used in process industries.
- Demonstrate the ability to apply basic concepts of Chemistry and Physics within process industries.
- Describe the importance of quality, safety, health and environment to the process industry.

Pre-requisites:
B.Sc. Chemistry background

Syllabus

Introduction
Classification of chemical industries, material of construction, process instrumentation, safety, fire protection and waste disposal. 0**3**

Acid industries
Manufacture, history, properties and uses of acetic acid, formic acid, benzoic acid, phthalic acid and oxalic acid. 0**5**

Fermentation industries
Introduction, culture development, inoculums preparation, nutrients for microorganism, toxic effects on culture. Manufacture, properties and uses of Industrial alcohol, absolute alcohol, butyl alcohol, glycerol, ethylene glycol and propylene glycol. 0**8**

Industrial sodium compounds
Manufacture, properties and uses of sodium thiosulfate, sodium bromide, sodium sulfate and sodium sulfite. 0**5**

Halogens and chlorinated compounds
Introduction, manufacture, properties and uses of fluorine, bromine, iodine, chlorine, methyl chloride, dichloromethane, chloroform and carbon tetrachloride. 0**7**

Electro-thermal industries
Introduction, classification and advantages of electric furnace. Manufacture of silicon carbide, calcium carbide, graphite and carbon electrodes. 04

Industrial solvents
Synthesis and properties of dimethylformamide (DMF), dimethyl sulfoxide (DMSO), tetrahydrofuran, dimethyl ether and diethyl ether. 0**4**

References:
1. P H Groggins, Unit processes in organic synthesis, 5th edition., Tata McGraw Hill Education (2004)
2. C.A. Heaton, An Introduction to Industrial Chemistry, Springer, 2014
3. G.T. Austin, Shreve's chemical process industries, 5th Edn., McGraw Publications - 2017
4. B. K. Sharma. Industrial chemistry, Goel publishing house 2014
5. G. N. Pandey, S. N. Srivastava, Fundamentals of Chemical Reaction Engineering, Galgotia Publications Pvt. Ltd. 2004

CHM 6012: Bioorganic and Medicinal Chemistry
[3-0-0-3]

Course Objectives:
At the end of this course students should be able to
- Understand, analyze and evaluate the chemistry of drugs and drug interactions
- Explain the principles of bioorganic and medicinal chemistry
- Describe pharmacological activity, structure-activity relationships and toxicity characteristics of certain drugs
- Discuss the principles of drug action, metabolism and stability

Pre-requisites:
B.Sc. Chemistry background

Syllabus
Bioorganic Fundamentals:
Nucleic acids: Nucleosides and nucleotides, structure and functions of DNA and RNA, *Proteins:* Classification, structure and properties of amino acids, classification, structure and properties of proteins, coagulation and denaturing of proteins, *Enzymes:* Naming and classification, Enzyme cofactors, Enzymes as catalysts, Factors affecting enzymatic reactions, Enzyme inhibition and specificity, *Lipids*: Structure, classification, distribution and biological importance, *Hormones*; Types and mechanism of action. 10

Biochemical Aspects:
Overview of metabolic processes – catabolism and anabolism, ATP- the biological energy currency, Biological membranes, Reaction mechanism of biochemical reactions associated with TPP, PLP, Energy value of the foods, Composition and detection of abnormal level of certain constituents leading to diagnosis. 06

Basic Medicinal Chemistry:
Definition and fundamental principles of drug therapy, Physiological properties of drug molecules in relation to biological activity: Solubility, partition coefficient, hydrogen bonding, chelation, pK_a values, geometrical and optical isomers, steric effect, redox potential. Principles of drug design: General principles of drug action and drug receptor interactions. 10

Applied Medicinal Chemistry:

Introduction, definition , classification, chemical nomenclature, brand names, synthesis of compounds, mechanism of action , uses and side effects of following classes of compounds: General anesthetics, Anticonvulsants, Antihistaminic agents, Analgesic agents, Antipyretic analgesics , Anti-inflammatory analgesics, Antibiotics, Antimalarials, Anti-hypertensives, Cardiovascular drugs, Antifertility drugs, Prostaglandins and Eicosanoids, Anticancer and Anti-HIV agents. 10

References:

1. A.L. Lehninger, *Principles of Biochemistry*, 5th Edn., Worth Publishers, New York, 2008
2. L. Stryer, W.H. Freeman, *Biochemistry,* 6th Edn., W.H. Freeman Company, New York, 2006
3. C.G. Wermuth Ed, *Medicinal Chemistry for 21st Century*, Oxford, Blackwell Scientific Publications, Oxford, 2001
4. M.E. Wolff, *Burger's Medicinal Chemistry and Drug Discovery*, Vol I , Principles and practice, 6th Edn., John Wiely and Sons, New York, 2003
5. A. Kar, *Medicinal Chemistry*, New Age Intl.(P) Ltd., New Delhi, 2006

CHM 6013: Computational Chemistry

[3-0-0-3]

Course Objectives:

At the end of the course students will be able to

- Propose the force fields to be applied to a given system
- Identify the ensembles to be used
- Apply the QM/MM methods to different branches of chemistry

Pre-requisites:

B.Sc. Chemistry background

Syllabus

Molecular Mechanics and Force Fields

Introduction to Molecular mechanics: Quantum mechanics and statistical mechanics, methods of calculations: Ab-iniitio, Semi-empirical methods.

Ab-initio method: Hartree - Fock method, Moller-Plesset perturbation theory, self-consistent field, quantum Monte Carlo method

Semi-empirical method: Complete Neglect of Differential Overlap (CNDO) - Austin Model 1 (AM1) and Parametric Model number 3 (PM3) methods

Density functional theory: local density approximation (LDA); generalized gradient approximation (GGA); Basis sets. 14

Molecular Simulation

Introduction, canonical ensembles: thermodynamics, perturbation theory, isobaric ensembles, isothermal-isobaric ensemble, grand canonical ensembles.
Monte Carlo Simulations: Metropolis Monte Carlo algorithm, Static and Dynamical properties of complex systems. 12

Combined QM/MM methods

Solvation and Solvent Effects, Application in organic, inorganic and organometallic systems. 10

References:

1. Christopher J. Cramer, Essentials of Computational Chemistry: Theories and Models, 2nd Ed., John Wiley & Sons, 2013
2. E. G. Lewars, Computational Chemistry: Introduction to the theory and applications of molecular quantum mechanics, 2nd Ed., Springer 2011
3. Alan Hinchliffe, Molecular Modelling for Beginners, 2nd Ed., John Wiley & Sons, 2011
4. David Young, Computational Chemistry: A Practical Guide for Applying Techniques to Real World Problems, John Wiley & Sons, 2004
5. Alan Hinchliffe, Chemical Modelling: Applications and Theory, Royal Society of Chemistry, 2008