DEPARTMENT OF CHEMISTRY

SCHEME OF INSTRUCTIONS AND SYLLABUS
(Course Book)
FOR

M.Sc in Chemistry

Visvesvaraya National Institute of Technology, Nagpur

July 2015
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1. General Information about the department

Science is basic foundation of any technological and engineering creation. In view of the changing scenario at national and international level in field of Science and Technology, there is great demand for basic sciences with considerable knowledge of its applications. VNIT is committed to high academic standards. The M.Sc. courses are designed for four semesters (two years) in such a way that a good basic foundation of subjects is laid and applications along with recent developments are covered. Relative grading will be followed and credits will be allotted based on academic performance. Students will also get theoretical and practical knowledge of computer programming. These M.Sc. programmes provide opportunity to make career in R&D, industries and academic institutions. Opportunity for the placement may be provided by the Institute.

2. Brief about M.Sc program:

Department of Chemistry offers M.Sc. (Chemistry) program which gives good foundation of basics and research component through practical skills, which in turn will provide excellent job prospects in Academics, Industries and other field of interest. M.Sc. (Chemistry) will provide competence to tackle frontier area in Green chemistry, supramolecular chemistry, Sensors, Advanced materials and Advanced organic chemistry. Two years M.Sc programme in Chemistry will be conducted in four semesters. Communication skill has been proposed as an audit course in first semester, which will help students develop better expression. In addition to theory and practical courses project phase-I and Computational chemistry lab will be introduced in third semester. Fourth semester has two elective courses, Basics of electronics and project phase-II. Nine electives have been incorporated in the course considering variety of advanced interest.

3. Details about Faculty members of Chemistry Department

<table>
<thead>
<tr>
<th>S.N.</th>
<th>Name</th>
<th>Qualification</th>
<th>E-mail ID</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Dr. Suresh S. Umare</td>
<td>Ph.D</td>
<td><a href="mailto:ssumare@chm.vnit.ac.in">ssumare@chm.vnit.ac.in</a> <a href="mailto:ssumare@rediffmail.com">ssumare@rediffmail.com</a></td>
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<td>Dr. Ramani V. Motghare</td>
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<td>6</td>
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<td>7</td>
<td>Dr. Atul V. Wankhade</td>
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<tr>
<td>8</td>
<td>Dr. Sangesh P. Zodape</td>
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<td><a href="mailto:szodape@chm.vnit.ac.in">szodape@chm.vnit.ac.in</a></td>
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<tr>
<td>9</td>
<td>Dr. Umesh R. Pratap</td>
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</tr>
<tr>
<td>10</td>
<td>Dr. Susanta Kumar</td>
<td>Ph.D</td>
<td><a href="mailto:sknayak@chm.vnit.ac.in">sknayak@chm.vnit.ac.in</a> <a href="mailto:nksusa@gmail.com">nksusa@gmail.com</a></td>
</tr>
<tr>
<td>11</td>
<td>Dr. Laxmi Gayatri</td>
<td>Ph.D</td>
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VISION AND MISSION
OF
DEPARTMENT OF CHEMISTRY

Vision

To establish the department as one of the best twenty chemistry programs in the country with acknowledged excellence in teaching and research at the nexus between basic science and applied science to serve the mankind and society.

Mission

1. To create and maintain the programs of excellence in the area of research, education and public outreach.
2. To promote, inspire and nurture the fundamentals of chemistry through UG & PG course offered for the science and applied science (engineering) students.
3. To offer research project with high emphasis on concept-theory-practical training in building up research interest for the transformation of budding chemists into productive scientist, excellent teacher and entrepreneur.
4. To become a nationally recognized centre of chemical sciences for modern education with a state of art centralized research facility.
## 4. CREDIT REQUIREMENTS FOR POST GRADUATE STUDIES

<table>
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<tr>
<th>Postgraduate Core (PC)</th>
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**Grand Total PC + PE** 63

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<tr>
<td>Chemistry of Advanced materials</td>
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<td>Supramolecular Chemistry</td>
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<td>Chemistry of Macromolecules</td>
<td>CHL 549</td>
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<tr>
<td>Photochemistry and Biophysical Spectroscopy</td>
<td>CHL 507</td>
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</table>
DETAILED SYLLABUS

SEMESTER I

CHL511 – MOLECULAR THERMODYNAMICS [(3-0-0); Credit: 3]

Objective:
To impart intensive and extensive knowledge of the subject enriching students to understand the role of Thermodynamic Chemistry in the field of science and engineering. To inculcate habit of scientific reasoning to do the task rationally. To develop skill and capabilities of students in solving problem of daily routine using thermodynamic and Statistical thermodynamic Chemistry in Life.

Outcome:
By the end of the course students gain insight to understand chemical and statistical thermodynamics aspects in chemical, biological and physical process in science and technologies.

Syllabus

Classical Thermodynamics, Review of Basic Classical Thermodynamics: The laws of thermodynamics, free energy, entropy, Partial molar quantities and chemical potential, real gases and fugacity.
Phase rule: Application to one, two and three component system
Molecular Partition Function: rotational, vibrational and translational partition functions.
Application: Equipartition Theorem, Debye and Einstien theory of heat capacity of solids and chemical equilibrium.

REFERENCES:
Objective:
The objective of the course is to encourage and prepare the students to cater the need of R&D activities of various chemical and pharmaceutical industries, by imparting detailed knowledge of important name reactions, oxidizing-reducing agents, selective organometallic reagents used in organic synthesis and their industrial applications.

Outcome:
By studying this course, the students will learn to design multi step synthesis and supposed to be capable to plan syntheses of organic molecules by proper choice of starting materials, reagents and reaction conditions.

Syllabus
Oxidation: Introduction, different oxidative processes: Chromium (VI) oxidants, Dimethyl sulfoxide, Swern Oxidation, Mangnese (IV) oxide, Silver carbonate, Oppenauer oxidation, Peroxide, peroxyacids, potassium permanganate, Osmium tetroxide, Prevost oxidation and Woodward modifications, Periodic acid, Lead Tetraacetate, NBS, DDQ, Chloranil, SeO₂.
Addition to Carbon – Hetero Multiple bonds: Addition of Grignard Reagent, Organo Zinc, Organo Copper, and Organo lithium reagents to Carbonyl and unsaturated Carbonyl compounds. Phosphorous, Nitrogen and Sulphur Ylids and their stereochemistry.

REFERENCES:
Objective:
Quantum Mechanics is a branch of science that deals with discrete, indivisible units of energy called quanta as described by the Quantum. It is an interfacial subject between Physics, chemistry and mathematics. Hence the objective of this course in chemistry is to understand clearly the microscopic and inner details of any reactions in chemistry viewpoint.

Outcome:
According to the student feedback for last three years this interfacial subject between Physics, chemistry and mathematics has provided a better scientific understanding and inner details of any physical or chemical reaction.

Syllabus

REFERENCES:
Objective: 
Objective of first part (Main group Chemistry) is to provide basic concepts on synthesis, structure, bonding and properties of some selected main group elements. Second part (Transition metal Chemistry) will be useful in building a conceptual framework for understanding the principles and theories that account for the physicochemical properties of coordination compounds.

Outcome:
Students will gain the fundamental knowledge about the synthesis, structure, bonding and properties of some selected main group elements. Exposure to the fundamental concepts on different theories of bonding and their relation to the properties of transition metal coordination compounds will be helpful in understanding the role of this class of compounds in different fields of application like in Organometallic Chemistry or Bioinorganic Chemistry for future study.

Syllabus
Main Group Chemistry: Synthesis, properties, structure and bonding in nitrogen, phosphorus, sulfur compounds, boranes, borazine, carboranes, silanes, silicates, silicones, iso and hetero polyanion
Synthesis and reactivity of organo-lithium, -beryllium and -magnesium –aluminium, germanium, tin and lead compounds
Chemistry of Ga(I) and In(I)
Inorganic chain, ring and cluster
Theories of bonding : VBT, CFT, d-orbital splitting in octahedral, JT-distorted octahedral, square planar, square pyramidal, trigonal bipyramidal, and tetrahedral complexes; CFSE, pairing energy, low-spin and high-spin complexes and magnetic properties; LFT, and molecular orbital (MO) theory of selected octahedral and tetrahedral complexes.
Electronic Spectra : UV-Vis, charge transfer, colors, intensities and origin of spectra, interpretation, term symbols and splitting of terms in free atoms, selection rules for electronic transitions, Orgel and Tanabe-Sugano diagram, Nephelauxetic series.
Magnetism: Types, magnetic susceptibility, spin only formula, spin-orbit coupling, spin cross over.Lanthanides and Actinides : contraction, coordination, optical spectra and magnetic properties.Reaction mechanisms: substitution reactions in octahedral and square planar complexes, trans effect and conjugate base mechanism, water exchange, anation and base hydrolysis, stereochemistry, inner and outer sphere electron transfer mechanism

REFERENCES:
CHP 526 - PHYSICAL CHEMISTRY LAB

Objective: To enable students to carry out, and interpret measurements within the context of the fundamental technological problem with which they are presented.

Outcome:
Student will acquire practical skills to perform, analyzes and optimize necessary process parameter in kinetic and thermodynamics processes.

Syllabus

Experiments on thermodynamics, kinetics, catalysis, spectroscopy and macromolecules.
To study Kinetics of inversion of cane sugar.
To study the reaction kinetics of hydrolysis of ethylacetate by NaOH.
To study the adsorption of Oxalic acid / acetic acid on Charcoal and verify Freundlich and Langmuir adsorption isotherm.
Study BET multilayer adsorption
Determination of partition Coefficient of iodine between organic solvent and water.
Determination of heat of ionization of acetic acid.
Determination of heat of Crystallization of Copper Sulphate
Determination of Molecular weight of a compound by Rast’s Camphor method.
Determine viscosity of oil using Redwood Viscometer.
Determine the critical micelle concentration of a soap( sodium laurate/ sodium palmitate, etc) by surface tension measurements (using stalagmometer)
Determination of refractive index of a liquid by Abbe refractometer and hence the specific and molar refraction.
To determine the specific and molecular rotation of an optically active substance.
Determination of partial molar volume of ethanol in dilute aqueous solution.

REFERENCES:

2. J.B. Yadav; Advance Practical Physical Chemistry; Goel Publishing House, 10th Edition.

CHP 516 - ORGANIC CHEMISTRY LAB.

Objective:
The aim and objective of the Organic practical course is to imbibe and develop practical skills, confidence and compliance for qualitative and quantitative analysis, preparation, separation techniques, isolation, extraction and characterizations using chemical and spectral and other
modern techniques. Besides, induce a vision to see the scope in R & D, self reliance through actual performance.

**Outcome:**

Students acquire all essential practical skills and learn techniques through Multistep preparations, estimations, extractions, separations, isolations, distillations, chemical and spectral characterization which provides deeper understanding of subject and confidence for implementation of newer ideas helping them to pursue higher education and R&D activities.

**Syllabus**

A. Separation and identification of two and three-component mixtures of organic compounds.

B. Preparation of organic compounds involving several stages and characterization of intermediates and final products. (Any 3)
   i) Phthalic anhydride → Phthallimide → Anthranilic acid.
   ii) Acetophenone → Oxime → Acetanillide.
   iii) Phthalic anhydride → o- benzoyl benzoic acid → anthraquinone.
   iv) Cyclohexanone → cyclohexanone oxime → caprolactone
   v) Anthranilic acid → o-chlorobenzoic acid → N-phenyl Anthranilic acid → acridone
   vi) Benzaldehyde → chalcone → chalcone epoxide
   vii) Benzophenone → benzopinacol → benzopinacolone

C. Separation / purification and characterization. (Any 2)
   a) Isolation of caffeine from tea leaves.
   b) Isolation of piperine from black pepper
   c) Isolation of β-carotene from carrots
   d) Isolation of lycopene from tomatoes
   e) Isolation of limonene from lemon peel
   f) Isolation of eugenol from cloves

D. Use of ultrasound and microwaves in organic synthesis. (Any 2)
   a) Ultrasound-assisted one-pot synthesis of 2,4,5-triarylimidazole catalyzed by ceric (IV) ammonium nitrate in aqueous media from benzaldehyde, benzil/benzoin and ammonium acetate.
   b) Synthesis of Benzotriazoles by Ultrasound Irradiation from o-phenylenediamine.
   c) The Hantzch dihydropyridine synthesis from aldehydes, ethyl acetoacetate and urea in microwave irradiation.
   d) Synthesis of coumarin by Knoevenagel synthesis using salicylaldehyde, ethyl acetate in presence of base in microwave irradiation.
   e) Synthesis of dihydropyrimidones from Biginelli Reaction by acid-catalyzed, three component reaction between an aldehyde, β-ketoester and urea.

**REFERENCES:**

Objective: Chemical kinetics is concerned with the study of the dynamics of chemical reactions. The raw data of chemical kinetics are the measurement of rates of reaction; the desired final product is the explanation of these rates in terms of complete reaction mechanisms. The objective of the present course is to introduce the foundation of the subject by studying series of reactions of increasing complexity and to show how experimentally measured parameters may be used to propose new models (mechanism) or verify existing models.

Outcome: This course will enable student calculate the rate of reaction, desired final product, yield of reaction and to understand the possible reaction mechanism.

Syllabus

REFERENCES:

1. Glasstone S.; Electrochemistry; Litton Educational pub.
Objective:
Primary aim of this course is to develop interest and skill for generating mechanistic path for organic transformations in the students. The focus of this course is to give the detailed insight of organic reaction mechanism and to understand the physical chemistry of organic reactions along with the stereochemistry of the reactants, intermediates and the products involved in an organic reaction.

Outcome:
After completion of the course students will understand the mechanistic pathways of the various organic reactions. Students will become competent to predict the chemo-, regio- and stereoselective outcome of such reactions.

Syllabus
Stereochemistry
Stereo chemical Principles – Enantiomeric relationships, diastereomeric relationships, R and S, E and Z nomenclature, dynamic stereochemistry, prochiral relationship, asymmetrical synthesis, stereo-specific and stereo selective reactions, three and erythro isomers. Introduction of optical activity in the absence of chiral carbon (biphenyls, spiranes, allenes and helical structures). Conformation of acyclic molecules and shape of six membered rings Stereochemistry and orientation of the addition to carbon-carbon multiple bonds. Stereochemistry of the compounds containing N, P and S.

Reaction mechanism
Definition of reaction mechanism, transition state theory, kinetics, qualitative picture. Substituent effects, linear free energy relationships, Hammett equation and related modifications. Basic mechanistic concepts like kinetic vs thermodynamic control, Hammond postulate, Curtin-Hammett principle, isotope effects, general and specific acid-base catalysis, and nucleophilic catalysis, reactive intermediates.

Aliphatic Nucleophilic Substitution
The SN2, SN1, mixed SN1 and SN2 and SET mechanism. The neighboring group mechanism, The Neighbouring group participation by $\pi$ & $\sigma$ bonds, Kinetic Isotope Effects, carbocation rearrangements in neighboring group participation. The SNi mechanism. Reactivity effects of structure, attacking Nucleophile, leaving group and reaction medium, Phase transfer catalyst, ambident nucleophile and regioselectivity. Aromatic Nucleophilic Substitution: SNAr, SN1 Benzyne & SNR1, Mechanisms, Reactivity effect of substrate structure, leaving group and attacking nucleophile.

Aromatic Electrophilic Substitution
Arenium ion mechanism, orientation and reactivity, energy profile diagram, The ortho/ para ratio ipso attack, orientation in other ring systems, Naphthalene, Anthracene, Six and five membered heterocycles, Diazonium coupling Vilsmeier reaction, Gattermann – Koch reaction, etc.

Elimination reactions
E2, E1, E1cb Mechanisms, Orientation, stereochemistry in elimination, reactivity effect of structure attacking and leaving groups, competition between substitution & elimination , syn eliminations.

REFERENCES:
CHL 523 - MODERN METHODS OF ANALYSIS

Objective:
To teach the proper use and importance of measurement statistics. To help students understand the theoretical aspects of various techniques used in chemical analysis like electro analytical methods, spectroscopy (absorption and emission), gravimetric, chromatographic separation and estimation etc. To stimulate the interest needed to approach research projects in new environments and to become familiar with the tools available.

Outcome:
On completion of the course, students acquire knowledge to select proper sampling procedures, techniques and instrumentation for particular sample analysis.

Syllabus
Sampling, statistical data treatment and evaluation of significant figures, error.
Instrumentation, Laboratory techniques and Analytical applications of the following:
Electroanalytical methods: Voltammetry, Coulometry, Amperometry, Potentiometry and Conductometry
Spectrometric methods I: UV-Visible and Atomic Absorption Spectroscopy.
Spectrometric methods II: IR spectroscopy, Atomic Emission Spectroscopy- Flame photometer.
Spectrometric methods III: Spectrofluorimeter, Spectrophosphorimeter, Raman effect, Raman spectrometer, NMR spectrometry.
Thermoanalytical: TGA, DTA, and DSC.
Separation techniques: Chromatography, Classification, Gas chromatography, GC-MS, High Performance Liquid Chromatography(HPLC), Ion Chromatography.
Mossebauer Spectroscopy: Mossebauer effect, recoilless emission and absorption, hyperfine interaction, chemical isomer shift, magnetic hyperfine and quadruple interaction and interpretation of spectra.
Electrophoresis (plate and capillary).

REFERENCES:
2. Day R.A; Underwood A.L; Quantitative Analysis (Sixth Edition); Prentice- Hall India; 2006
3. Willard, Merritt, Dean, Settle; Instrumental Methods of Analysis, 7th edition; CBS Pub,

CHL 524 - ORGANOMETALLICS AND CATALYSIS [(3-0-0); Credit: 3]

Objective:
First part (Organometallics) is designed to provide the basic knowledge of organometallic chemistry with reference to synthesis, structures, bonding, reactivity and application of organometallic compounds. Second part (Catalysis) deals with role of various catalysts, their mechanism and application in different fields.

Outcome:
Students will learn the basic features of organometallic compounds, catalytic process and their reactions, which are very important for different application.

Syllabus

General Introduction: Valence electron count (16/18 electron rules); Types of M-C bonds
Structure and bonding in mono and polynuclear metal carbonyls; substituted metal carbonyls, nitrosyls, alkyls, allyls, and cyclopentadienyl derivatives
Synthesis and reactivity of metal alkyls, carbenes, carbines, alkenes, alkynes, and arene complexes; metallocenes and bent metallocenes; isolobal analogy
Reaction of organometallic compounds: substitution, oxidative addition, reductive elimination, insertion, disinsertion, polymerization
Catalysis: Physisorption, Chemisorption, Homogenous and Heterogenous catalysis, Biocatalysis, Catalysis and green chemistry
Photo Catalysis: Photo catalysis and the environment, water purification, organic and pollutant degradation, self cleaning, reactors for photo catalysis

REFERENCES:

2. R. C. Mehrotra and A. Singh, Organometallic Chemistry, A Unified Approach, New Age International
5. Gadi Rothenberg, Catalysis Concept and Green Applications, First edition, Wiley-VCH
Objective:
To teach proper solution handling, preparation of standard solutions, use appropriate calibration methods, be familiar with the correct use of volumetric glassware and to become familiar with good laboratory practice (GLP) and the development of standard operating procedures (SOPs). Provide a basic understanding of the principles, instrumentation and applications of chemical analysis.

Outcome: The students develop skill and capabilities to perform quantitative instrumental analysis.

Syllabus

Potentiometry
1. To determine weight of hydrochloric acid and acetic acid in a given mixture of acid solution by potentiometric titration (Using Quinhydrone).
2. Determination of dissociation constant of a weak acid by EMF method.

Conductometry
3. Determine the cell constant of a given conductivity cell using 0.1N KCl solution and determine the strength of HCl and CH₃COOH by conductometric titration.
4. Determination of dissociations constant of weak acid conductometrically.

Spectrophotometry
5. Determine $\lambda_{\text{max}}$ and verify Beer's-Lambeurt's law for KMnO₄ and K₂Cr₂O₇ solutions.
6. Spectrophotometric determination of the $pK_a$ of an indicator (the acid dissociation constants of methyl orange).
7. Analysis by UV-Visible spectrophotometer.
8. Analysis by flame photometer.
9. Analysis by AAS.

Ion-exchange
10. To separate cobalt and Nickel on anion exchange resin & determination of weight recovered.

Chromatography
11. Analysis by HPLC.

REFERENCES
2. Galen W. Ewing; Instrumental Methods of Chemical Analysis, Fifth edition; McGraw-Hill Book Company,

CHP 515 - INORGANIC CHEMISTRY LAB

Objective:
This course will help in developing practical skill with reference to synthesis and studies of some properties, qualitative and quantitative analysis of inorganic compounds.

Outcome:
Students will have hands on training in developing the skills related to qualitative and quantitative inorganic analysis.
Syllabus

1. Analyses of Ores & Alloys (Any two of the followings)
   (i) Gravimetric Analysis of Ni in Ni-Steel
   (ii) Volumetric Analysis of Cu and Zn in Brass
   (iii) Complexometric Analysis of mixtures of cations

2. Preparation of Inorganic compounds/ complexes and Characterization: (Any three of the followings)
   Reinecke’s Salt, [Ni(en)$_3$]Cl$_2$, [Co(en)$_3$]Cl$_3$, Dibenzyltin(IV)chloride, Tris(oxalate) manganese(III), Tris(acetylacetonato) iron(III), Tris(2,2’-bipyridine)ruthenium(II) perchlorate

3. Semi-micro Inorganic Qualitative Analyses
   For Qualitative analysis following cations, anions, insoluble salts, Special elements will be included.
   Determination of ions and composition of the salt to be predicted by chemical analysis.
   Cations: Na, K, NH$_4$, Al, Cr, Mn, Fe, Co, Ni, Cu, Zn, Cd, Hg, Ag, Pb, Sn, As, Mg, Ca, Ba, Sr
   Anions: F, Cl, Br, I, SCN$, S^{2-}$, SO$_4^{2-}$, SO$_3^{2-}$, S$_2$O$_3^{2-}$, P$^\text{V}$, As$^\text{V}$, Si$^{IV}$,
   Special Elements: Be, Th, U, Ce, V, Mo, W, Zr, Ti

4. Studies on composition of complexes in following systems by Job’s, Mole ratio and Slope ratio methods (Any one of the followings)
   i) Cu(II)-ethylene diamine
   ii) Fe(III)- sulphasalysilic acid
   iii) Fe-1,10 phenanthroline compounds

REFERENCES:


SEMESTER – III

CHL531- APPLICATION OF SPECTROSCOPIC TECHNIQUES FOR STRUCTURE DETERMINATION [(3-0-0); Credit: 3]

Objective:
The objective of the course is to help students understand the theoretical aspects of various spectroscopic techniques like UV-Visible, IR, NMR and Mass, which in turn, will enhance their capability of interpreting the spectral data obtained from various techniques and use it for structural elucidation of organic compounds.

Outcome:
Students acquire the knowledge of the instrumentation and principle involved in various advanced spectroscopic and will be able to interpret the spectral data for structural elucidation of organic compounds.
Syllabus

UV-Vis Spectroscopy: Fieser-Woodward rules for conjugated dienes and carbonyl compounds, Fieser-Kuhn rules for polyenes. UV spectra of aromatic compounds and heteroaromatic compounds. Calculation of $\lambda_{\text{max}}$ for the benzene derivatives.


NMR Spectroscopy (Organic): 1H NMR: General introduction and definitions, Chemical shift, Spin-spin interaction, shielding mechanism of measurement of chemical shift values and correlation for protons bonded to carbon and other nuclei. Factors affecting chemical shift. Deuterium exchange. Spin-spin coupling, factors affecting coupling constant. Simplification of complex spectra, nuclear magnetic double resonance, contact shift reagents, solvent effects. Fourier transform technique. Nuclear Over-Hauser effect (NOE). Resonance of other nuclei; F$^{19}$ and P$^{31}$. C$^{13}$ NMR: Resolution and multiplicity of 13C NMR, 1H-decoupling, noise decoupling, broad band decoupling; NOE signal enhancement, off-resonance, proton decoupling, applications of CMR. DEPT; Introduction to 2D-NMR: COSY, NOESY, DEPT, INPET, APT, INADEQUATE.

Mass Spectroscopy: Theory, instrumentation and modifications; Unit mass and molecular ions; Important terms- singly and doubly charged ions, metastable peak, base peak, isotropic mass peaks, relative intensity, FTMS, etc.; Recognition of M+ ion peak; General fragmentation rules. McLafferty rearrangement. Structure elucidation problems using the above spectroscopic techniques.

REFERENCE:


CHL 532 - SOLID STATE AND SURFACE CHEMISTRY [(3-0-0); Credit: 3]

Objective:

To understand the synthesis, structure, properties and application of solid state materials.

Outcome:

This course is very useful to learn structure-properties of materials with the understanding of the structures, morphology of the materials through techniques like X-ray diffraction, SEM and
TEM. It will be also useful to familiar with the Electrical, Magnetic and Optical properties of solid state materials.

**Syllabus**

Crystal Structure: Crystalline and amorphous solids; Crystal systems, Point groups, Space groups and Crystal structure, Methods of characterization of crystal Structure - Powder X-ray diffraction, electron and neutron diffraction; Types of close packing - Hexagonal close packing (HCP) and Cubic close packing, Packing efficiency, Radius ratios; Description of solids: Crystal Structure Types – Rock salt, Sphalerite, Antifluorite, Wurtzite, rutile and, Perovskit, Spinels. Preparative Methods: Solid state reaction, Co-precipitation as precursor, Crystallization of solutions, glass, melts and gels. Intercalation / Deintercalation reactions, Ion-exchange reactions. Methods of Single Crystal Growth: Solution growth; Melt Growth-Bridgman, Kyropoulos, Verneuil; Chemical vapour transport; Fused salt electrolysis; Hydrothermal method. Electrical, Magnetic and Optical Properties: Band theory of solids - Metals and their properties; Semiconductors - Extrinsic and intrinsic, Hall effect; Thermoelectric effects (Thomson, Peltier and Seebeck); Insulators - Dielectric, Ferroelectric, Pyroelectric and Piezoelectric properties; Ionic conductors. Dia, Para, Ferro, Ferri, and Antiferro Magnetic types; soft and hard magnetic materials; select magnetic materials such as spinels, garnets and perovskites, Hexaferrites and Lanthanide-transition metal compounds; Magnetoresistance. Luminescence of d- and f- block ions; structural probes: up and down conversion materials. Superconductivity: Basics, discovery and high Tc materials. Microscopic techniques: Scanning electron microscope (SEM), Transmission electron microscope, electron spectroscopy for chemical analysis (ESCA).

**REFERENCES:**


**CHL 533 - BIOINORGANIC CHEMISTRY**

[3-0-0]; Credit: 3

**Objective:**

This course is framed to provide an in depth understanding of some important aspects of metal ions in biological system.

**Outcome:**

Learning the important role of metal ions in biological systems will create interest to pursue research work in related field.

**Syllabus**

General Introduction: Essential and trace elements, Biological importance of inorganic elements Function and transport of K\(^+\), Na\(^+\), Ca\(^{2+}\), Mg\(^{2+}\) in biological system Active site structure and functions of:

Electron transfer proteins - ferredoxin, rubridoxin and cytochromes.
Metal ion transport and storage protein - Ferritin, Transferrin, Siderophores and metallothionein
Oxygen transport and storage protein - Hemoglobin, myoglobin, hemerythrin, hemocyanin
Oxygen activation protein – Catalase, peroxidase, superoxide dismutase cytochrome P450, cytochrome C oxidase, ascorbic oxidase
Other metalloenzymes: Zn enzyme- Carbonic anhydrase and carboxypeptidase, Co coenzyme - vitamin B12
Nitrogen fixation: Nitrogenases

REFERENCES:

2. W. Kaim and B. Schwederski, Bioinorganic chemistry: Inorganic Elements in the Chemistry of Life, John-Wiley & Sons

CHP 534 - COMPUTATIONAL CHEMISTRY LAB. [(0-0-2); Credit: 1]

Objective:
To provide hand on experience on use of various software’s available for Chemistry.

Outcome:
The main outcome of this essential lab course is to provide the platform to the student to be skilled in molecular modeling, docking and with other computational chemistry softwares that are needed for higher studies.

Syllabus
Draw the structure of simple aliphatic, aromatic, heterocyclic compounds with different substituent. Get the correct IUPAC name and predict the H1NMR signals.
Use of MS-WORD, Power point, Excel and origin software for treatment of experimental data, X-Y plot, plotting bar graph, statistical analysis in chemistry, Use of Internet for literature survey, handling scifinder, Scopus and other search engine.
Structure elucidation using Software (mass spectra)
Computer programming; Exposure to available standard packages like SPSS, Chemdraw, PC Model, MOTECH, TURBOMOLE, MOLPRO, MOLCAS, MM2 and Gaussian.

REFERENCE:

1. G.Grant and W. Richards, Computational Chemistry, Oxford University press.
CHP 535 - SYNTHEIS AND CHARACTERIZATION LAB. [(0-0-6); Credit: 3]

Objective:
This laboratory course will introduce students an appreciation for the synthesis and different characterizations of composites and nano materials.

Outcome:
Students learn the synthetic techniques of polymeric and nano-materials and have ability to analyze and interpret the characterization data relevant to their structure/performance. They will also be familiar with some of the modern instrumental techniques.

Syllabus
1. Synthesis and properties exploration of Polyaniline
2. Synthesis and properties exploration of Phenol-formaldehyde resin
3. Synthesis and studies of superadsorbent polymer
4. Molecular weight determination of polymers
5. Synthesis and characterization of metal oxide nanoparticles
6. Thermal decomposition of CaCO₃
7. Determination of Tₑ and Tₘ of polymers
8. Study of electrical conductivity of polymeric materials
9. Studies of mechanical properties
10. Rheological studies of polymeric materials

REFERENCES:

CHP536 - PROJECT PHASE – I [(0-0-6); Credit: 3]
SEMESTER-IV

ELECTIVE I and II

CHL541-CHEMISTRY OF ADVANCED MATERIAL [(3-0-0); Credit: 3]

Objective:
This course is framed to provide an in depth understanding of some important aspects of advanced materials and their applications.

Outcome:
After completion of the course students will acquire the fundamental knowledge, which will develop their interest on different advanced materials, their properties and applications.

Syllabus

Metal and Alloys: Properties and application of iron, nickel, copper, chromium, aluminium and their alloys

Polymer: Synthesis, properties and application of UHMWPE, PEEK, ABS, Polysyloxane, polysilanes, biopolymer

Ceramics: Refractories : Classification of Refractories, Basic raw materials, properties and areas of application; Glass: Definition of glass, Basic concepts of glass structure, Different types of glasses. Application of glasses


Composites: Definition of composite materials; classification: particulate and dispersion hardened composites, continuous and discontinuous fibre reinforced composites, metal-matrix composites, carbon-carbon composites, molecular composites, micro-and multilayer composites, theory of reinforcement; Effect of orientation and adhesion.

REFERENCES:

1. C N R Rao, Chemistry of advanced materials, Blackwell Publishing Ltd
4. Alain Nouailhat, An Introduction To Nanosciences And Nanotechnology, John wiley and sons
CHL542-CHEMISTRY AND TECHNOLOGY OF WATER [(3-0-0); Credit: 3]

**Objective:** To impart knowledge and experience in water testing for a better understanding of drinking and industrial water characteristics.

**Outcome:**
This course will help students understand the problems and solutions related to drinking and industrial water.

**Syllabus**

Water quality, impurities, effects and removal. WHO and BIS guidelines for Drinking water. Treatment for domestic and industrial purpose. Water quality index and inter-relation between water quality parameters. Characteristics of waste water, Constituents in waste water, constituents of concern, sampling and analytical procedures, physical constituents, inorganic non-metallic constituents, metallic constituents, aggregate organic constituents (measurement of BOD, COD, SCOD, TOC, DTOC etc), individual organic compounds, biological characteristics, microorganisms found in surface water and waste water. Introduction to process analysis and selection. Physical unit operations, chemical unit process, fundamentals of biological treatment, disinfection process, water reuse.

**REFERENCES:**

2. Mamta Tomar; Quality Assessment of Water and Waste Water; CRC Pr. I Llc; May 1999

CHL543-SENSORS AND CHEMICAL SENSORS [(3-0-0); Credit: 3]

**Objective:**

Identification and development of the appropriate surface science tools. To extend understanding of complex phenomena of chemical sensing and sensor-molecule interactions on functionalized surfaces have sensitive structures.

**Outcome:**
At the end of the course student will be able to understand the different sensing technologies used for various important applications.
Syllabus

Introduction to sensors, Transduction elements- Electrochemical transducers Potentiometry and ion selective electrodes, Voltametry and Amperometry, Field effect transistors, Modified electrodes, Thin film and Screen printed electrodes, photometric sensors.


Performance factors: selectivity, sensitivity, response time, recovery time, life times, Precision, Accuracy and Repeatability.

Basic principle, Instrumentation and application of Mass sensitive and Thermal sensor, optical sensors, Potentiometric Biosensors.

REFERENCES:

1. Brain R. Eggin; Chemical Sensors Bio sensors; Wiley India Pvt. Ltd, 2002
2. R. A. Potyrailo, Vladimir M. Mirsky; Combination Method for Chemical and Biological Sensors; Springer, 2009

CHL544-GREEN CHEMISTRY AND SUSTAINABILITY [(3-0-0); Credit: 3]

Objective:
To understand the development and new approaches for designing of safer chemical process & product without causing harm to the environment and human life.

Outcome:
Students will acquire the fundamental knowledge about the innovative approaches for designing of safer chemical products, processes and use of renewable resources for sustainable development.

Syllabus


Evaluation of Environmental Performance During Process Synthesis: Environmental performance tools – Economic criteria, environmental criteria, Threshold limit values, permissible exposure limits, and Recommended exposure limits, Toxicity weighting; evaluating alternative synthetic pathways; Life cycle assessment, HAZOPs.


REFERENCES:

3. Anastas P.T. and Williamson T.C.; Green Chemistry, Frontiers in Benign

CHL545-PERCYCLIC REACTION AND PHOTOCHEMISTRY [(3-0-0); Credit: 3]

Objective: 
This course is framed to provide an in depth understanding of some important aspects of pericyclic reactions and photochemistry.

Outcome: 
On the completion of the course students will have the understanding of basics of organic Photochemistry and Pericyclic reactions. Various theories/rules governing these pericyclic reactions will help them to predict the products with stereochemistry involved in these reactions.

Syllabus
Pericyclic reactions: Classification, electrocyclic, sigmatropic, cycloaddition and ene reactions, Woodward-Hoffmann rules, and FMO theory, perturbation of molecular orbital (PMO) approach of pericyclic reaction under photochemical condition, Claisen, Cope, Sommelet-Hauser, and Diels-Alder reactions in synthesis, stereochemical aspects.


Photochemistry of alkenes and related compounds : Isomerization, Di-π-methane rearrangement and cycloadditions.

Photochemistry of aromatic compounds : Ring isomerization and cyclization reactions.

CHL546-CHEMISTRY OF HETEROCYCLIC COMPOUNDS [(3-0-0); Credit: 3]

Objective:
This course is framed to provide an in depth understanding of some important aspects of heterocyclic compounds and organometallic compounds.

Outcome:
Student will understand the significance of heterocyclic compounds in day to day life as well as in biological systems and drug synthesis. This course makes student capable to design multi-step synthesis for heterocyclic compounds of moderate complexity using conceptual models and retro-synthetic analysis strategies.

Syllabus

General Considerations: The Disconnection Approach and Retrosynthesis.

The Chemistry of: (i) Three-membered rings-Aziridines, (ii) Four-membered rings- Azetidines and their 2-Oxo derivatives, (iii) Condensed pyrroles- Indoles, (iv) Azoles- Oxazoles, isoxazoles, pyrazoles, imidazoles and thiazoles, (v) Six-membered rings- Pyrimidines and purines. Structure and synthesis of Caffeine. Reagents and Reactions: Principle, Preparation and applications of the following reagents and reactions with mechanistic details: Grignard reagents, Organolithium reagents, Organoboron reagents: hydroboration, reactions of organoboranes in C-C bond formation. Gilman’s Reagent (Lithium Dimethyl cuprate), Lithium Diisopropylamide (LDA), Trimethylsilyl iodide, Diazomethane, 1,3-Dithiane (Umpolung reagent), Polyphosphoric acid, DCC (Dicyclohexylcarbodiimide), Peterson’s synthesis, Bakers yeast, Organophosphorus compounds (Wittig reaction), Phase transfer catalysts: Quaternary ammonium and phosphonium salts, Crown ethers, Heck reaction, Suzuki coupling, Mukaiyama reaction.

REFERENCES:

CHL547-SUPRAMOLECULAR CHEMISTRY [(3-0-0); Credit: 3]

Objective:

Supramolecular chemistry refers to the area of chemistry beyond the molecules and focuses on the chemical systems made up of a discrete number of assembled molecular subunits or components. While traditional chemistry focuses on the covalent bond, supramolecular chemistry examines the weaker and reversible non-covalent interactions between molecules. The study of non-covalent interactions is crucial to understanding many biological processes from cell structure to vision that rely on these forces for structure and function. Biological systems are often the inspiration for supramolecular research.

Outcome:

Students will acquire the concepts of supramolecular chemistry and will get insight of fundamental interactions and their applications in living organisms and in complexation of compounds. New trends in designing supramolecular complexes and devices.

Syllabus


Synthesis and structure of crown ethers, lariat ethers, podands, cryptands, spherands, calixarenes, cyclodextrins, cyclophanes, cryptophanes, carcerands and hemicarcerands.

Host-Guest interactions, pre-organization and complimentarity, lock and key analogy. Binding of cationic, anionic, ion pair and neutral guest molecules.

Crystal engineering: role of H-bonding and other weak interactions.

Self-assembly molecules: design, synthesis and properties of the molecules, self assembling by H-bonding, metal-ligand interactions and other weak interactions, metallomacrocycles, catenanes, rotaxanes, helicates and knots.

Molecular devices: molecular electronic devices, molecular wires, molecular rectifiers, molecular switches, molecular logic.

Relevance of supramolecular chemistry to mimic biological systems: cyclodextrins as enzyme mimics, ion channel mimics, supramolecular catalysis etc.

Examples of recent developments in supramolecular chemistry from current literature. Chemistry and photophysics of porphyrins and ruthenium polypyridine complexes: photodynamic therapy (PDT), electrogenerated chemiluminescence (ECL)
REFERENCES:

5. J.D. Seader, E.J. Henly, Introduction to soft mater Synthetic and Biological self assembly materials, Separation process principles: 2nd edition Willy.

CHL548-BIOMOLECULES

Objective: To provide an in depth understanding of some important aspects of compounds.

Outcome:
Student will have the knowledge of natural molecules and their interactions and physiological roles.

Syllabus

Lipids and membranes: Classification of lipids, self-association of lipids-micelles, reverse micelles and membranes, transport of cations through membranes.
Carbohydrates: Oligosaccharides and polysaccharides, role of sugars in biological recognition.
Metabolism and Energetics: Catabolic and anabolic processes, glycolysis, citric acid cycle and oxidative phosphorylation.
Enzyme: Enzyme kinetics and applications of enzymes in organic synthesis. Principles of enzyme inhibition, implications in drug design
Molecular recognition: Chiral recognition, supramolecular chemistry, and hydrogen bonding in molecular organization. PCR techniques

REFERENCES:


CHL549-CHEMISTRY OF MACROMOLECULES

Objective:
To provide an in depth understanding of some important aspects of Polymers.

Outcome:
Students will learn and able to describe the physical aspect of structure, characteristic and behavior of various macromolecule.
Syllabus

Basic Concepts: Structure of polymers- linear, branched, cross linked, classifications of polymer, stereo regular polymer- Atactic, Syndiotactic and Isotactic, Molecular weights, Molecular weight distribution, Number average, Weight average, Viscosity average molecular weight and Methods of determination: GPC, Intrinsic-viscosity, Mark-Houwinks relationship, Chemistry of thermoplastic and thermoset polymers, Degree of crystallinity.


Polymer Processing and Rheology: Calendering, Extrusion, Molding, Coating, Fiber spinning. Rheometric characterization of polymer solution and melts.

Polymer Structure-Property Relationships: Effect of chemical composition on various properties of polymer, Mechanical properties: stress-stain in polymers, elasticity, tensile strength; Transition properties: T_g, T_m ; Electrical properties: Electrical conductivity, Dielectric constant, power factor, dissipation factor; Optical properties; Chemical properties: Cohesive energy, solubility, polymer toxicity; Physical properties of polymers and adhesives.

Engineering and Specialty Polymers (Preparation, Properties and Applications): Polyolefin’s; Polyamide; Biopolymers; Insulating polymers; Inorganic polymers (Polyphosphazenes, Polysilanes, Polysiloxanes); Conducting polymers, Liquid-Crystal polymers, Ionic polymers, PEEK, PTFE, Phenolic & Epoxy Resin.


REFERENCES:


CHL 507-Photochemistry and Biophysical Spectroscopy [(3-0-0); Credit 3]

Objective:

This is an advanced level course designed to understand the mechanism of absorption of light and its interaction with matter and its consequences. A proper understanding of the process is essential before one can start photochemical reactions.

Outcome:

This advance level course will enable student to understand the microscopic details of consequences of absorption of light and its interaction with matter in the field of photophysics and photochemistry.
Syllabus

Introducing photochemistry:
Importance of photochemistry, Laws of photochemistry, Photochemistry and spectroscopy, Nature of light & nature of matter, Interaction between light and matter, Electronic energy states of atoms, The selection rules

Diatomic and polyatomic molecules:
Mechanism of absorption and emission of radiation of photochemical interest, Electric dipole transitions, Einstein treatment of absorption and emission phenomenon, Life times of excited electronic states of atoms and molecules, Types of electronic transitions in organic molecules

Physical properties of electronically excited molecules:
Nature of changes on electronic excitation, Electronic, vibrational and rotational energies, Potential energy diagram, Shapes of absorption band and Frank condon principle, Emission spectra, Environmental effect on absorption and emission spectra, Excited state dipole moment, Excited states acidity constants- pK values, Excited state redox potential, Emission of polarized luminescence, Geometry of electronically excited molecules

Photophysical processes in electronically excited molecules:
Types of photophysical pathways, Radiationless transition- Internal conversion and intersystem crossing, Fluorescence emission, Fluorescence and structure, Triplet states and phosphorescence emission, Emission property and the electronic configuration, Photophysical kinetics of unimolecular processes, State diagrams, Delayed fluorescence, The effect of temperature on emission process

Photophysical kinetics of bimolecular processes:
Kinetic collisions and optical collision, Bimolecular collision in gases and the mechanism of fluorescence quenching, Collisions in solutions, Kinetics of collisional quenching: Stern Volmer equation, Concentration dependence of quenching and excimer formation, Quenching by foreign substances, Some aspects of Organic and Inorganic Photochemistry, Chemiluminescence

Protein Fluorescence:
Spectral Properties of the Aromatic Amino Acids:
Excitation Polarization Spectra of Tyrosine and Tryptophan, Solvent Effects on Tryptophan Emission Spectra, Excited-State Ionization of Tyrosine, Tyrosinate Emission from Proteins

General Features of Protein Fluorescence:
Tryptophan Emission in an Apolar Protein Environment, Energy Transfer and Intrinsic Protein Fluorescence, Tyrosine-to-Tryptophan Energy Transfer in Interferon-γ, Quantitation of RET Efficiencies in Proteins, Phenylalanine-to-Tyrosine Energy Transfer

REFERENCES:

PROJECT PHASE – II [0-0-8]; Credit: 4]