DEPARTMENT OF CHEMISTRY
SCHOOL OF PHYSICAL AND MATHEMATICAL SCIENCES
UNIVERSITY OF KERALA

M.Sc. Programme in Chemistry
Syllabus
(Under Credit and Semester System w. e. f 2017 Admission)
DEPARTMENT OF CHEMISTRY
SCHOOL OF PHYSICAL AND MATHEMATICAL SCIENCES
UNIVERSITY OF KERALA

M.Sc. PROGRAMME IN CHEMISTRY

Programme Objectives

• To raise the academic and intellectual standards of the student in such a way that after the completion of the programme the student will be equipped with knowledge in various topics in chemistry both in basic and advanced levels.

• To train the students to improve their practical knowledge during the first three semesters and to impart special practical skills depending on the work they choose for their dissertation in fourth semester.

• To pave way for overall development of students by providing ground for improving their leadership qualities, communication skills, extra-curricular abilities, interpersonal relationships and civic sense.

• To mould the students so that they can be competent enough in order to clear national and international level examinations which determine their career.

• To groom the students to become responsible citizens to serve the nation.
Structure of the Programme

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<th>Semester No.</th>
<th>Course code</th>
<th>Name of the Course</th>
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<td>CHE-E-443 (iii)</td>
<td>Electronic Structure Theory and Applications</td>
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<td>CHE-E-443 (iv)</td>
<td>Photophysical Processes and Applications</td>
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Extra Departmental Electives Offered by the Department

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* The students have to take 3 extra department elective courses of 2 credits each (one from inside school and two from outside and obtain a total of 72 credits.)
AIM: To familiarize the students with the basic concepts in inorganic and bio-inorganic chemistry

OBJECTIVES

- To introduce coordination chemistry and its significance
- To make the students understand the inorganic chemistry in biological systems
- To enable students to build concept on the properties of inorganic compounds under various pH and in non-aqueous condition.

COURSE CONTENT


MODULE II: Theories of Structure and Bonding in Metal Complexes: Valence bond theory and its limitations. Ligand field theory: Splitting of d orbitals in different ligand fields such as octahedral, tetragonal, square planar, tetrahedral, trigonal bipyramidal and square pyramidal fields. Jahn-Teller effect. LFSE and its calculation. Thermodynamic effects of LFSE. Factors affecting the splitting parameter. Spectrochemical series. Molecular orbital theory based on group theoretical approach and bonding in metal complexes. MO diagrams of complexes with and without π bonds. Effect of π bond on the stability of σ bond. Sigma and pi bonding ligands such as CO, NO, CN⁻, R₃P, and Ar₃P. Nephelauxetic series.


MODULE VI: Chemistry of noble gases: Early chemistry, Xenon fluorides and oxofluorides; Synthesis, properties, structure and bonding. Xenon compounds with bonds to other elements. Chemistry of Krypton and Radon. Chemistry of halogens: Halogens in positive oxidation states. Interhalogen compounds, pseudohalogens and polyhalide ions including polyiodide anions. Astatine.

REFERENCES

ADDITIONAL REFERENCES

SEMESTER: I
COURSE CODE: CHE-C-412
COURSE TITLE: ORGANIC CHEMISTRY I
CREDITS: 3

AIM: To equip the students with fundamental concepts in organic chemistry

OBJECTIVES

- To train the students in the art of writing organic reaction mechanism
- To enable the student to view molecules understanding their stereochemistry
- Stereochemical implications on addition, substitution, elimination and rearrangement reactions

COURSE CONTENT

MODULE I: Structural Organic Chemistry - Aromaticity, Hückel’s rule, criteria for aromaticity, annulenes, mesoionic compounds, metallocenes, cyclic carbocations and carbanions, anti- and homo- aromatic systems, Fullerenes, Carbon nanotubes and graphenes, Physical organic chemistry - kinetic and thermodynamic control of reactions, Hammond’s postulate, kinetic isotope effects with examples, linear free energy relationships, Hammett and Taft equations, Catalysis by acids and bases with examples like acetal, cyanohydrin, ester formations and hydrolysis reactions, Acidity and Basicity of organic compounds, pKa values, kinetic and thermodynamic acidity. Hard and soft acids and bases - HSAB principle and its applications.

MODULE III: Reactions of sp³ Carbons - Stereochemical and mechanistic aspects of S_n reactions, Effect of solvent, leaving group and substrate structure, Neighbouring group participation, Non-classical carbocations and ion pairs in S_n reactions, Ambident nucleophiles and substrates, S_n' and S_n,i reactions, Isotopic and salt effects, Elimination reactions leading to C=C bond formation. E1, E2 and E1CB mechanisms, Hoffman and Saytzeff modes of elimination, Effect of leaving group and substrate structure, Pyrolytic eliminations – Chugaev and Cope eliminations, Cis eliminations. Substitution vs elimination.

MODULE IV: Reactions of sp² Carbon and Aromatic Systems - Electrophilic addition to C=C, Mechanistic and stereochemical aspects of bromine addition, halolactonization, hydrogenations, hydroborations, epoxidation including Sharpless asymmetric epoxidation, hydroxylations including Woodward-Prevost hydroxylations, oxy-mercuration and de-mercuration and singlet carbene addition. Stereochemistry of addition to C=O systems. Cram's rule and Felkin-Anh Model. Aromatic electrophilic and nucleophilic substitutions, Electronic and steric effects of substituents. S_n1, S_nAr, Benzyne and S_n1 mechanism and their evidences.

MODULE V: Reactions of carbonyl compounds - Aldol and mixed-aldol condensations, Claisen, Reformatsky, Perkin, Stobbe, Darzens, Knoevenagel, Dieckmann, Thorpe, Henry and Mannich reactions, reductions of carbonyl group (Clemmenson and Wolff-Kishner), Addition of cyanide, ammonia, alcohol and Grignard reagents, Structure, synthesis and reactions of α,β – unsaturated carbonyl compounds, Michael addition and Robinson annulation, Prins reaction.

REFERENCES


ADDITIONAL REFERENCES

- Kalsi, P. S. "Stereochemistry and Reaction Mechanisms", Wiley Eastern, 1993,

************
AIM: To equip the students with an in-depth knowledge in Quantum Mechanics, Group Theory and Surface Chemistry.

OBJECTIVE

- To train the students in exactly solving the Schrodinger equation for simple systems.
- To provide an in-depth analysis on the beautiful concept of symmetry and point groups.
- To familiarize the students with the fundamentals of surface chemistry.

COURSE CONTENT


MODULE II: Exactly solvable problems: Solutions of Schrodinger wave equations for:


MODULE III: Schrodinger equation in polar coordinates and exactly solvable problems: Solutions of Schrodinger wave equations for


MODULE VI: Colloids- zeta potential, electrokinetic phenomena, sedimentation potential and streaming potential, Donnan membrane equilibrium. Emulsions: macro- and micro-emulsions; aging and stabilization of emulsions; Phase behaviour of microemulsions. Surface Enhanced Raman Scattering, Surfaces for SERS studies, Chemical enhancement mechanism, Surface selection rules, Applications of SERS. Application of low energy electron diffraction and photoelectron spectroscopy, ESCA and Auger electron spectroscopy, scanning probe microscopy, ion scattering, SEM and TEM in the study of surfaces.

REFERENCES

- Gregg S. J., “The Surface Chemistry of Solids”, Chapman Hall.

ADDITIONAL REFERENCES

- Ramakrishnan V. and Gopinathan M. S., ”Group Theory in Chemistry”, Vishal Publications.

************
AIM: To enable the students to master both qualitative and quantitative analysis

OBJECTIVES

- To enable the students to practice separations of metal ions and identifications
- To enable the students to master the art of volumetric estimations

COURSE CONTENT

MODULE I: Separation and identification of rare/less familiar metal ions such as Ti, W, Se, Mo, Ce, Th, Zr, V, U and Li in their binary mixtures. A student must analyse at least 6 samples.

MODULE II: Quantitative volumetric estimations of various metal ions using EDTA.

MODULE III: Volumetric quantitative estimations using ammonium vanadate.

MODULE IV: Volumetric quantitative estimations using cerium (IV) sulphate (Cerimetry).

MODULE V: Quantitative volumetric estimations using chloramine-T.

MODULE VI: Volumetric quantitative estimations using potassium iodate.

A student must do a total of at least 8 volumetric estimations.
REFERENCES:

- Vogel, A. I. "A Text Book of Qualitative Inorganic Analysis", Longman.

**********
AIM: To enable the students to practice organic separations by solvent extraction

OBJECTIVES

- To impart hands-on training in organic binary mixture separations using ether extraction and identification of the separated compounds
- To enable the students to practice thin layer chromatography

COURSE CONTENT

MODULE I: Quantitative wet chemistry separation of a mixture of two components by solvent extraction using ether. Separation of acidic component from basic component. Identification of the separated compounds

MODULE II: Separation of acidic/basic component from neutral component. Identification of the separated compounds by functional group analysis,

MODULE III: Preparation of derivatives for acidic, basic and neutral components like esters, anhydrides, amides, picrates, hydrazones etc

MODULE IV: Separation by distillation method. Ordinary distillation and vacuum distillation, Separation by sublimation and crystallization methods.

MODULE V: Separation of binary mixtures of organic compounds using TLC. Identification using $R_f$ values, Identification of number of products in a reaction mixture, different methods for TLC visualization
**MODULE VI:** Separation of binary mixtures by column chromatography. Packing a column, loading of sample and elution. TLC visualization and removal of the solvent to collect the pure fraction, Demonstration of HPLC technique.

**REFERENCES**


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SEMESTER:   I
COURSE CODE:  CHE-C-416
COURSE TITLE:  PHYSICAL CHEMISTRY LAB I
CREDITS:   2

AIM: To familiarize the students with experiments to appreciate the ideas from distribution law, chemical kinetics, thermochemistry, adsorption and refractive index.

OBJECTIVES

- To enable the students to appreciate the distribution law, kinetics and adsorption.
- To familiarize the students in using instruments such as refractometer, and polarimeter

COURSE CONTENT


MODULE II: Refractometry: Refractive index and molar refraction of liquids. Atomic refractions. Composition of solid solutes. Molecular and ionic radii from molar refraction. Study of the complex $K_2\text{[HgI}_4\text{]}$.


**REFERENCES**

- Daniels, F. and Mathews, J. H. "Experimental Physical Chemistry", Longman.
- James, A. M. "Practical Physical Chemistry", Churchill.
SECOND SEMESTER

(SEMESTER: II)

(COURSE CODE: CHE-C-421)

(COURSE TITLE: INORGANIC CHEMISTRY II)

CREDITS: 3

AIM: To enable the students to master the properties of metal complexes and various aspects of organometallic chemistry

OBJECTIVES

- To help the students learn the spectral and magnetic properties of metal complexes
- To help the students understand the stability and reactivity of metal complexes
- To enable the students to master basic aspects of organometallic chemistry

COURSE CONTENT


MODULE IV: Coordination Chemistry of Lanthanides and Actinides: General characteristics of lanthanides-Electronic configuration, Term symbols for lanthanide ions, Oxidation state, Lanthanide contraction. Factors that mitigate against the formation of lanthanide complexes. Electronic spectra and magnetic properties of lanthanide complexes. Lanthanide complexes as shift reagents. General characteristics of actinides-difference between 4f and 5f orbitals, comparative account of coordination chemistry of lanthanides and actinides with special reference to electronic spectra and magnetic properties.


REFERENCES:


ADDITIONAL REFERENCES:

- Crabtree, R. H. "The Organometallic Chemistry of Transition Metals", 2Edn, Wiley.
- Wilkins, R. G. "Kinetics &Mechanism of Reactions of Transition Metal Complexes", 2Ed, VCH.

************
AIM: To familiarize the students with radical chemistry and its applications, concerted reactions and organic spectroscopy

OBJECTIVES

- To enable the students to understand about free-radical and photochemical reactions
- To enable the students to identify the type of pericyclic reaction and to suggest mechanism for the same
- To train the students in the art of identifying molecules based on spectroscopic data

COURSE CONTENT

MODULE I: Radicals in Organic Synthesis - Structure, stability and generation of free radicals, Baldwin’s rules of ring closure, Inter and intramolecular additions of radicals to alkenes and alkynes, Radical chain reactions, Introduction to polymers and free-radical polymerizations, Named reactions – Pinacol, acyloin, McMurry, Hoffmann-Löfler-Freytag and Barton reactions, Use of NBS and tributyl tin hydrides, , Ullmann coupling.


MODULE IV: NMR Spectroscopy - Magnetic nuclei with emphasis on $^1$H and $^{13}$C, shielding, de-shielding and chemical shifts, factors affecting chemical shifts - Field and anisotropic factors, relaxation processes, chemical and magnetic non-equivalence. $^1$H and $^{13}$C NMR scales, Spin-spin splitting – AX, AX$_2$, AX$_3$, AB, ABC and AMX type coupling, Coupling constants.. Pascals triangle, first order and non-first order spectra, Karplus curve, Quadrupole broadening, virtual and long-range coupling, Shift reagents and their role, Decoupling and double resonance, Off-resonance decoupling, NOE.

Introduction to 2D NMR. Correlation, NOE and quantum correlation spectroscopy techniques like COSY, HETCOR, HMQC, HMBC, NOESY and EXCY.

Selective population inversion – DEPT, INEPT and RINEPT, Sensitivity enhancement and spectral editing, MRI Problems on spectral interpretation.

MODULE V: UV-Vis and IR Techniques - UV-VIS spectra of enes, eneones, arenes and conjugated systems. Woodward-Fieser rules, Solvent effect on absorption spectra. Chiroptical properties – introduction to CD and ORD, Cotton effect, octant rule, axial haloketone rule. Characteristic IR bands of functional groups. Factors affecting the IR stretching frequency – vibrational coupling, hydrogen bonding, electronic, inductive and field effects, Identification of functional groups and other structural features by IR.

MODULE VI: MS in organic structure analysis. EI, CI, SIMS, FAB, ES and MALDI ion production methods. Characteristic EIMS fragmentation modes and MS rearrangements including McLafferty rearrangement., Spectral interpretation, structure identification and solving of structural problems using numerical and spectral data.

REFERENCES

ADDITIONAL REFERENCES

- Wayne, C. E. and Wayne, R. P. “Photochemistry”, OU Primer 39, OUP.

************
AIM: To familiarize the students with quantum mechanical approach of chemical bonding, and to equip them with physical theories of spectroscopy.

OBJECTIVES

- To provide the students with various approximations incorporated in solving the Schrodinger equation of many body problems
- To provide an in-depth knowledge in physical principles of IR, Raman, UV-Visible, NMR and ESR spectroscopy

COURSE CONTENT


REFERENCES


ADDITIONAL REFERENCES

- Atkins P. W., "Physical Chemistry", OUP.

************
SEMESTER: II
COURSE CODE: CHE-C-424
COURSE TITLE: INORGANIC CHEMISTRY LAB II
CREDITS: 2

AIM: To help students master the quantitative separation and analysis of metal ion mixtures. To get hands on training in colourimetry.

OBJECTIVES

- To enable the students to learn estimation of inorganic mixtures.
- To master alloy analysis and colorimetric estimation of metal ions

COURSE CONTENT

MODULE I: Colorimetric determination and estimation of Iron, after plotting calibration graph.

MODULE II: Quantitative estimation of Chromium, by colorimetry.

MODULE III: Colorimetric estimation of Nickel, after plotting calibration graph.

 MODULE IV: Quatitative colorimetric determination of Manganese.

MODULE V: Colorimetric estimations of Ti, W and Cu., after plotting calibration graph.

MODULE VI: Estimation of simple binary mixtures of metal ions in solution (involving quantitative separation) by volumetric and gravimetric methods.
REFERENCES:


************
AIM: To give hands-on-training for the students to set up organic reactions, isolate the product and characterize them using spectroscopic techniques

OBJECTIVES

- To enable the students to practice setting up of organic reactions and monitoring
- To apply the spectroscopy which they learn in the theory classes

COURSE CONTENT

MODULE I: Preparation of organic compounds by single step reactions – benzoylation, esterification, nitration, sulphonation, halogenation and hydrolysis

MODULE II: Preparation of compounds by double-stage synthesis – nitration followed by hydrolysis, bromination followed by hydrolysis etc

MODULE III: Reactions of carbonyl compounds – aldol condensation – preparation of chalcones and oximes

MODULE IV: Preparation of heterocyclic compounds - benzimidazoles, thiazoles and N-alkylated isatins.
MODULE V: Spectral interpretation of organic compounds [simple as well as those prepared in lab as above] using UV-VIS and IR, NMR analysis of compounds

MODULE VI: Recording the UV-Vis and IR spectra of synthesized compounds

REFERENCES

- Furniss, B. S and others, “Vogel’s Textbook of Practical Organic Chemistry”, ELBS.
SEMESTER: II
COURSE CODE: CHE-C-426
COURSE TITLE: PHYSICAL CHEMISTRY LAB II
CREDITS: 2

AIM: To provide the students with hands-on training and get themselves expertise in physical chemistry experiments from various areas such as viscosity, surface tension, phase equilibria, cryoscopy and transition temperatures

OBJECTIVES

- To enable the students to perform experiments from various areas such as viscosity, surface tension, cryoscopy, phase equilibria, transition temperature
- To enable the student to find out the unknown composition using viscosity and surface tension methods, and from eutectic diagram

COURSE CONTENT


MODULE II: Surface tension: Surface tension and parachor of liquids by differential capillary and stalagmometer methods. Variation of surface tension with concentration. Determination of atomic parachor.


MODULE V: Phase equilibria II: Construction of Two component eutectic diagrams, determination of unknown concentration of given mixture. Three component systems with one pair of partially miscible liquids. Construction of phase diagrams and tie lines. Composition of homogeneous mixtures.


REFERENCES

- Daniels, F. and Mathews, J. H. "Experimental Physical Chemistry", Longman.
- James, A. M. "Practical Physical Chemistry", J. A. Churchill.

************
AIM: To enable the students to master the theories about structure and properties of solid state inorganic compounds and various chain, ring, cage and cluster inorganic materials.

OBJECTIVES

- To provide a ground knowledge about theories and properties of solid state materials
- To provide an insight about the chemistry of open and closed structure compounds of important non-metallic elements
- To introduce the concept of the structure and properties of various metallic clusters

COURSE CONTENT


MODULE IV: Structures of Sulphur, Nitrogen, Phosphorus and Silicone Compounds: Sulphur-Nitrogen compounds: Tetrasulphur tetranitride, disulphur dinitride and polythiazyl. $S_N$ compounds. S-N cations and anions. Other S-N compounds. Sulphur-phosphorus compounds: Molecular sulphides such as $P_4S_3$, $P_4S_7$, $P_4S_9$ and $P_4S_{10}$. Phosphorus-nitrogen compounds: Phosphazenes. Cyclo and linear phosphazenes. Other P-N compounds. Silanes, silicon halides, silicates; Classification and structure, silicones.


MODULE VI: Other Metal clusters: Factors favouring metal-metal bonds, Dinuclear compounds of Re, Cu and Cr, metal-metal multiple bonding in (Re$_2$X_8)$^{2-}$, trinuclear clusters, tetranuclear clusters, hexanuclear clusters. Carbonyl clusters-LNCCS and HNCCS, Isoelectronic and isolobal analogy, Wade-Mingos rules, cluster valence electrons. Polyatomic zintl anion and cations. Infinite metal chains. Isopoly acids of vanadium, molybdenum and tungsten. Heteropoly acids of Mo and W.

REFERENCES:

ADDITIONAL REFERENCES


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AIM: To develop the organic synthetic skills of the student and introduce him to various aspects of bioorganic chemistry

OBJECTIVES

- To introduce to the students the various synthetic reagents used in organic chemistry
- To introduce them to the large world of natural product chemistry
- To give them knowledge about synthetic and bio-polymers, their synthesis, structure and reactivity

COURSE CONTENT

MODULE I: Construction of Carbocyclic and Heterocyclic Rings - Importance of heterocyclic compounds, Structure and aromaticity of heterocycles, Trivial and Systematic Hantzsch Widman Nomenclature of heterocyclic compounds, Different methods of ring synthesis, Three and four membered heterocycles, Named reactions for synthesis of furan, pyrrole, thiophene, pyridine, indole, quinoline and isoquinoline including Paal-Knorr, Feist-Benary, Fischer indole, Hantzsch, Skraup, Pictet-Spengler and Bischler-Napieralski methods, Electrophilic and nucleophilic substitutions of 5-membered, 6-membered, indole, quinoline and isoquinoline rings, Heterocycles with more than one heteroatom – synthesis and reactivity. Pauson-Khand reaction, Volhardt reaction, Bergman cyclization, Nazarov cyclization, Olefin metathesis.

MODULE II: Organic Synthetic Strategies - Introduction to retrosynthetic analysis. Linear and convergent synthesis, Synthons, functional group interconversions (FGI), Role of protecting groups in organic synthesis, Enolate and enamine alkylation reactions including Stork-enamine reaction, Dipole inversion - Umpolung. Organometallic reagents like Grignard, alkyl lithium and Gilman Reagents and their utility, Organocuprates, DABCO and Baylis-Hilman reaction, Role of palladium in organic synthesis, Heck, Sonogashira, Suzuki, Stille and Negishi coupling reactions. Glaser coupling, Tebbe olefination, Sakurai reaction, Brook rearrangement, Mitsunobu reaction, $\text{PPh}_3\text{CBr}_4$ reagent
MODULE III: Reagents for oxidation - Oxidations using manganese and chromium reagents, PCC, PDC Collins and Jones reagents, Etard reaction, Use of SeO₂, MnO₂, Ag₂CO₃ and lead tetraacetate, DMSO based reagents - Swern oxidation, Oppenauer oxidation. Oxidation of alkenes - OsO₄, RuO₄, HIO₄, ozone and peracids. Sharpless asymmetric epoxidation, Woodward and Prevost hydroxylations, Dehydrogenation to aromatic compounds. Baeyer-Villiger oxidation, Dakin reaction.


MODULE V: Natural Products Chemistry - Classification, Isolation, identification, typical examples and structures of secondary metabolites - Alkaloids, Terpenoids, Steroids, Prostaglandins, Coumarins and flavones. Degradation methods for structural elucidation – Hoffmann and Emde methods, examples of alkaloids, Total synthesis of reserpine, Classification of terpenes, Cationic rearrangements and formation of cyclic terpenes, Structural elucidation of santonin, Structure and importance of quercetin; β-carotene and ascorbic acid. Synthesis of Vitamin C from glucose, Biosynthesis of fatty acids and polyketides by acetate pathway, monoterpenes by mevalonic acid pathway and alkaloids by shikimic acid pathway, biosynthesis of higher terpenes and steroids. Structure of cholesterol and other important steroids, Barbier Wielander degradation and Blanc rule

MODULE VI: Chemistry of nucleic acids and proteins - Amino acids, proteins and peptides: Structures and synthesis of amino acids – Strecker synthesis, Azlactone synthesis and enantioselective synthesis. Reactions of amino acids due to the NH₂ group, COOH group and its reaction with ninhydrin, Structure of proteins, Introduction to enzyme and co-enzymes, structure and relevance of NAD, chymotrypsin, pyridoxal and thiamine, Peptide bond formation methods, amino and carboxy protection in SPPS. ADP and ATP. Automated polypeptide and oligonucleotide synthesis. Structure of polysaccharides including starch, cellulose, glycogen and chitin.
REFERENCES

- Hanson, J. R “Organic Synthetic Methods” RSC, 2002.
- Hanson, J. R. “Natural Products: Secondary Metabolites”, RSC
- Mann, J and others, “Natural Products: Chemistry and Biological Significance”. Longman 2006

ADDITIONAL REFERENCES

- Harbourne, J. B. “Phytochemical Methods” Chapman Hall.
- Krishnaswamy, N. K. “The Chemistry of Natural Products,” Universities Press 2010
- Mann, J. “Chemical Aspects of Biosynthesis”, Oxford primer 20, OUP 1994
- Simmonds, R. J. "Chemistry of Biomolecules", RSC. 1992

************
AIM: To provide an in-depth knowledge in classical and statistical thermodynamics, chemical kinetics and electrochemistry.

OBJECTIVE

- To provide a good understanding in classical and statistical thermodynamics and its important derivations.
- To familiarize the students with thermal and photochemical reactions and related rate theories
- To familiarize the students with the fundamentals of electrochemistry.

COURSE CONTENT


REFERENCES

- Panchenkov G. M. and Labadev V. P., "Chemical Kinetics and Catalysis", MIR Publishing.

ADDITIONAL REFERENCES

- Atkins P. W., “Physical Chemistry”, OUP.

************
AIM: To master the preparation and characterization of metal complexes, to gain experience in the analysis of ore and fertilizer.

OBJECTIVES

- To apply the analysis techniques which was done in 1 and 2 sems in real cases
- To apply the theories of complexes by synthesizing and characterizing them

COURSE CONTENT

MODULE I: Analysis of some typical alloys such as brass, bronze and type metal.

MODULE II: Analysis of some typical ores: Carbonate ore, sulfate ore, ilmenite and monazite.

MODULE III: Analysis of fertilizers: Estimation of nitrogen in ammonium compounds. NPK estimations in synthetic fertilizers

MODULE IV: Ion exchange separation of binary mixtures: Zn & Mg and Co & Ni.

MODULE V: Preparation of various transition metal complexes

MODULE VI: Characterizations of prepared metal complexes by UV-VIS, IR, magnetic susceptibility and electrical conductivity
REFERENCES

- Palmer, W. G. "Experimental Inorganic Chemistry", CUP.
- Schoder, W. R. and Powell, A. R. "Analysis of Minerals and Ores of Rare Elements".
- Weining, I. and Schoder, W. P. "Technical Methods of Ore Analysis".

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SEMESTER: III
COURSE CODE: CHE-C-435
COURSE TITLE: ORGANIC CHEMISTRY LAB III
CREDITS: 2

AIM: To impart hands-on-training for functional group analysis of organic compounds

OBJECTIVES

- To apply volumetric analysis for functional group estimation in organic compounds
- To apply the UV-VIS spectroscopic technique for estimation of certain compounds

COURSE CONTENT

MODULE I: Estimation of esters and acids using acid-base titration method

 MODULE II: Estimation of reducing sugars by using freshly prepared Fehling’s solution

 MODULE III: Estimation of phenols, amines and ketones using iodometric titration method

 MODULE IV: Estimation of acid value, iodine value and sap value of oils

 MODULE V: Spectrophotometric estimation of total ascorbic acid content in various fruits and vegetables

 MODULE VI: Spectrophotometric estimation of glucose
REFERENCES

- Agarwala, A. C. and Sharma, R. M. "A Laboratory Manual of Milk Inspection", Asia Publishing
SEMESTER : III
COURSE CODE: CHE-E-437 (I)
COURSE TITLE: ADVANCED INORGANIC CHEMISTRY
CREDITS : 3

AIM: To enable the students to master the various advanced topics in nuclear chemistry. This course also helps the students to identify research problems in the active R&D areas in inorganic synthesis, spectroscopy and photochemistry.

OBJECTIVES

- To give an idea about advanced topics in nuclear chemistry, inorganic synthesis and photochemistry
- To cover advanced topics about inorganic materials used in real world applications

COURSE CONTENT


MODULE II: Inorganic synthesis: Special techniques such as chemical vacuum line, plasmas, photochemical apparatus and electrolysis. Synthesis of transition metal complexes involving the following methods: Electron transfer reaction, substitution reaction, reactions of coordinated ligands, aldol condensation, imine bromination hydrolysis, substituent exchange reaction, template effect and macrocyclic ligands. Complexes with interlocking ring ligands. Formation of supramolecular species.

MODULE IV: ESR and Mössbauer spectroscopy of coordination compounds: ESR spectra of metal complexes- hyperfine splitting, g values, zero field splitting and Kramers degeneracy. Application of ESR spectroscopy in the structural investigation of copper(II) and manganese(II) complexes. Mössbauer spectroscopy- Mössbauer effect, hyperfine interactions, isomer shift, electric quadrupole and magnetic hyperfine interactions. Application of Mössbauer spectroscopy in the structural study of iron and tin complexes.


MODULE VI: Chemistry of Materials: Glasses, ceramics, composites, nanomaterials-preparative procedures. Sol-gel synthesis, glassy state-glass formers and glass modifiers, ceramic structures, mechanical properties, clay products, refractories- characterizations, properties and applications. Radiopharmaceuticals (Tc). Ultramarines, zeolites and Metal organic frameworks (MOF); Synthesis structure and applications.
REFERENCES:

- Wilkins, R. G. “Kinetics & Mechanism of Reactions of Transition Metal Complexes”, 2nd Edn, VCH.

ADDITIONAL REFERENCES


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AIM: To introduce to the students certain advanced topics in organic chemistry

OBJECTIVES

- To make the students realize about the varied applications of organic chemistry
- To introduce the students to five different areas of advanced organic chemistry
- To introduce to the students the important areas of organic application research

COURSE CONTENT


MODULE III: Medicinal Chemistry and the Chemistry of the Cell - Introduction to drug discovery and design, drug administration, Drug action – pharmacokinetic and pharmacodynamic phases, modeling techniques, receptor proteins, drug receptor interaction, drug action, drug selectivity, drug metabolism, Classification of drugs, Anti-anginal drugs, antihypertensive agents, antimalarial drugs, aminoquinolines, Antibiotics and analgesics with examples. Drug stability,
Penicillins, tetracyclins and cephalosporins. Drugs for cancer, AIDS and diabetes, Composition and structural features of lipids.


**MODULE V:** Chemistry of Biomolecules - Primary structure determination of peptides, proteins and nucleic acids, DNA replication, Codon and anticodon recognition. Protein biosynthesis, transcription and translation, Genetic code, regulation of gene expression, DNA sequencing. The Human Genome Project. DNA profiling and the Polymerase Chain Reaction (PCR).


**REFERENCES**


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AIM: To equip the student with an in-depth knowledge on the advances in certain developing fields of physical chemistry such as industrial catalysis, photochemistry, computational chemistry and energy storage systems.

OBJECTIVES

- To familiarize the students with developing areas such as industrial catalysis, energy storage systems and computational chemistry
- To provide a detailed understanding on corrosion and protective coating.
- To appreciate the aforementioned fields by providing suitable applications and examples.

COURSE CONTENT

MODULE I: Surface area and porosity measurement. Preparation of catalysts, Precursor compound, Preactivation and activation process. Basic steps of phase transfer catalyzed reactions, transfer and intrinsic rates of catalysis.


**MODULE III:** Protective Coatings: Paints: Constituents, functions & mechanism of drying. Varnishes and Lacquers; surface preparation for metallic coatings, electroplating (gold) and electrode less plating (Nickel), anodizing, phosphate coating, powder coating & antifouling coating. Laser assisted surface engineering, Micro-Arc oxidation, Electro-spark coating.


REFERENCES

- Environmental Management-Vijay Kulkarni & Ramachandran T V., Teri Press, New Delhi, 2009
SEMESTER : III
COURSE CODE: CHE-L-436
COURSE TITLE: PHYSICAL CHEMISTRY LAB III
CREDITS : 2

AIM: To provide the students with hands-on training and get themselves expertise in certain instrumental methods such as conductometry, potentiometry, polarography, flame photometry and Karl-Fischer titrator. The students will also be introduced to the use of computers in Chemistry.

OBJECTIVES

- To enable the students to perform physical experiments using conductometer, potentiometer, polarpgraphic method, flame photometric method and Karl-Fischer titrator.
- To enable the students to use computers in Chemistry either by learning to write simple programs in C++ or by learning to use softwares to do molecular modeling and computations.

COURSE CONTENT


MODULE IV: Flame photometry: Estimation of Na⁺, K⁺, Li⁺, Ca²⁺ and Mg²⁺. Composition of the mixtures.

MODULE V: Karl-Fischer titrator: Estimation of water contents in pharmaceuticals, oils, fats and paints.
MODULE VI: Computers in Chemistry: Writing, compiling, and executing a computer program in C++, for any four chemical problems given: Determination of molecular weight of an organic compound, Determination of decay constant, half life and average life of a radioactive element, Calculating the normality/molarity/molality of a given solution, Calculating the pH of a solution.

OR

Calculate the equilibrium geometry, geometrical parameters and energy of molecules: water, methane, ethane, acetone, and acetaldehyde using MOPAC semi empirical program.

REFERENCES


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FOURTH SEMESTER

SEMESTER : IV
COURSE CODE : CHE-E-443 (v)
COURSE TITLE: ORGANIC SYNTHESIS
CREDITS : 4

AIM: To familiarize the students with advanced aspects of organic synthesis

OBJECTIVES

- To make the student well-versed in the art of organic synthesis via the retrosynthesis approach
- To introduce some modern synthetic tools with reference to recent research globally

COURSE CONTENT

MODULE I: The Disconnection Approach - Designing a synthesis, FGI, Synthons, order of events, choosing a disconnection, synthesis of aromatic compounds, chemoselectivity in synthesis – one group C-X disconnections – alcohols, ethers, sulphides, alkyl halides, two group C-X disconnections, 1,1- and 1,2- C-C disconnections, one group C-C disconnections, enolate chemistry, two-group disconnections, 1,1-, 1,2-, 1,3-, 1,4- and 1,5- difunctionalized compounds.

MODULE II: Retrosynthesis in Action - Advanced strategies, retrosynthesis in industry, stereoselectivity and regioselectivity in synthesis, using alkenes, alkynes and nitro compounds in synthesis, reconnections, retrosynthetic analysis and synthesis – practice problems, Synthesis of longifolene and Corey lactone.

MODULE III: Heterocyclic Ring Synthesis - Three, four, five and six membered ring synthesis and retrosynthesis, aromatic heterocycles, aromatic heterocycles with two heteroatoms, rearrangements in synthesis, electrophilic substitution reactions, named reactions in heterocyclic synthesis.

**MODULE V:** Asymmetric Synthesis - Organocatalysis, Prolines and NHCs – synthesis and reactivity, Transition metal mediated reactions in organic synthesis, Olefin metathesis, Grubbs catalysts, Enantiomers and diastereomers. resolution methods, Stereospecific and stereoselective synthesis, Asymmetric Synthesis - Principles, General strategies, Chiral Pool strategy, Chiral Auxiliaries, Asymmetric Diels Alder Reaction, Chiral Reagents – Binol Derivatives of LiAlH₄, Chiral Catalysts – CBS Catalyst.

**MODULE VI:** Reagents – Use of DDQ, iodobenzene diacetate, CAN, manganese acetate, FeCl₃, NMO, Dess Martin periodinane, SmI₂, N-heterocyclic carbenes, Na tetracarbonyl ferrate, benzenetricarbonyl chromium: TEMED, TEMPO, TMS, CBr₄ + Ph₃P

**REFERENCES**

AIM: To introduce analytical principles and environmental chemistry in a general manner

OBJECTIVES

- To introduce data analysis and error calculations
- To introduce certain instrumental techniques
- To introduce and explain the relevance of environmental chemistry

COURSE CONTENT


MODULE III: Basis and procedure of sampling, sampling statistics, sampling liquids, gas and solids(metals and alloys), preparation of a laboratory sample, moisture in samples, determination of water, Karl Fischer Method. Decomposition and dissolution, source of error, reagents for decomposition and dissolution, microwave decompositions, combustion methods, use of fluxes. Elimination of interference from samples-separation by precipitation, electrolytic precipitation, extraction and ion exchange. Distribution ratio and completeness of multiple extractions. Types of extraction procedures.

MODULE IV: Analytical procedures involved in the environmental monitoring of water quality- BOD, COD, DO, nitrite and nitrate, iron, fluoride, soil moisture, salinity, soil colloids, cation and anion exchange capacity. Air pollution monitoring: Control measures for air pollutants. sampling and collection of air pollutants-SO₂, NO₂, NH₃, O₃, and SPM. Principle of the analysis of milk and starch based food materials, Analysis of drugs, oils and fats.


REFERENCES

- Jeffery, G.H. Bassett, J. Mendham, J. Denney, R. C. Vogel's Text Book of
- Van Loon, G. W. “Environmental Chemistry”, OUP.
- Wilson, C. L. and Wilson, D. W. “Comprehensive Analytical Chemistry”, Vol. IB.

ADDITIONAL REFERENCES


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AIM: This course intends to provide fundamental insight to various instrumental analytical techniques by explaining their theory, principle and instrumentation.

OBJECTIVES

- To introduce the students to the various methods of instrumental analysis
- To give an understanding about the theory, principle and instrumentation of various analytical instruments

COURSE CONTENT


MODULE II: Chromatographic Methods Principles, instrumentation and applications of column chromatography, paper chromatography, thinlayer chromatography, ion-exchange chromatography, Gas chromatography and HPLC. Detectors, Hyphenated techniques, Capillary Electrophoresis, Introduction to Chiral Chromatography, Molecular Exclusion Chromatography, Affinity Chromatography. Introduction to Method development and Analysis of samples using the above techniques.


MODULE IV: Electroanalytical Methods Principles, instrumentation and applications of Electrogravimetry, Coulometry, Polarography, Amperometry, Cyclic voltametry, Potentiometry and Conductometry. Analysis of samples using the above instruments.

MODULE V: Thermal and Surface Analysis Methods Principles, instrumentation and applications of thermogravimetry (TG), derivative thermogravimetry (DTG), differential thermal analysis (DTA) and differential scanning calorimetry (DSC). Analysis of samples using the above instruments, Introduction to SEM, TEM, AFM and other surface characterization techniques.

REFERENCES


ADDITIONAL REFERENCES

- Fifield, F.W. Kealey, D. Principles and Practice of Analytical Chemistry, Blackwell

************
AIM: To train the student in some particular area according to his or her aptitude

OBJECTIVES

- To familiarize the student with the research area
- To introduce the student to most essential research equipments/softwares
- To train the student to write a report, present the results and think in-depth

DISSERTATION

The student is to work under the guidance of a supervising teacher and do experimental or theoretical work / part of a research work as suggested by the Supervisor and finally present his work and submit a report.

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AIM: To familiarize the students with the various industrial applications of chemistry

OBJECTIVES
- To make students aware about the chemical industry
- To bring light into the day to day relation of chemistry with human life

COURSE CONTENT


REFERENCES

- Baird, C “Environmental Chemistry”, Publisher WH Freeman, 2008
- Kumar, R & Singh, R N “Municipal water and waste water treatment”, Teri Press, 2008
- Patwardhan, I A D “Industrial Solid Wastes”, Teri Press, New Delhi, 2012

ADDITIONAL REFERENCES

- De, A. K. “Environmental Chemistry”
- Sharma, B. K. “Industrial Chemistry”, Goel publishing house, Meerut.

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AIM: Intended to provide advanced insight into major aspects of nanomaterials and their application.

OBJECTIVES

- To introduce nanomaterial synthesis, properties and applications
- To impart knowledge about molecular interactions in nanoscale and nanoarchitectures

COURSE CONTENT


MODULE II: Chemical Interaction at Nanoscale - Interparticle interactions in nanoscale, Types of intermolecular bonding, Electrostatic interactions, Ion pair interactions, solvent effects, ion dipole and dipole dipole interactions, Dative bond, π-interactions hydrogen bonding, Van der waals attractions and its physical property dependence, hydrophobic effect, Ostwald ripening. Reverse micelle as Spherical nanoreactors.

MODULE III: Nanostructured Molecular Architectures - Carbon fullerenes, its structure and applications, Superconductivity in C_{60}. Carbon nanotubes, its structure, electrical and mechanical properties and applications. Semiconductor nanomaterials, Graphenes, Carbon dots, Dendrimers. Biological nanomaterials, biomimetics, Self assembly of proteins, micelles and vesicles. Liposomes Core shell structures, Ferrofluids.

MODULE IV: Synthesis, of Nanomaterials - Solution based synthesis of nano particles, Synthesis of quantum dots, silver and gold nanoparticles using aqueous chemical method, Brief introduction to vapour phase synthesis of nanoparticles, Introduction to Physical vapour deposition, Molecular beam epitaxy, Chemical vapour deposition, Chemical beam Epitaxy, Atomic layer deposition,


REFERENCES

- Pradeep T., “Nano the essentials, Understanding Nanoscience and Technology”, McGraw – Hill
- Prasad, P M “Nanophotonics” John Wiley and Sons, New Jersey, 2004

ADDITIONAL REFERENCES:

- DiVentra, M., Evoy, S and Heflin, Jr, J. R. (Editors). “Introduction to Nanoscale Science and Technology, Publisher: Springer
- Klabunde, K. J. (Editor), “Nanoscale Materials in Chemistry,”
- Settle, F., Handbook of Instrumental Techniques for Analytical Chemistry,

************
AIM: To provide a detailed understanding of various computational strategies adopted to uncover the electronic structure of molecules

OBJECTIVES

- To familiarize the students with wave function based and density based electronic structure theory methods
- To provide a detailed understanding on molecular mechanics and simulations
- To provide an experience in modeling molecules and performing optimizations

COURSE CONTENT


MODULE III: Basis sets and Basis functions. Slater type orbital (STO) and Gaussian type orbital (GTO). Contracted and primitive. Basis sets. Minimal, multiple zeta, split-valence, polarized and diffused. Pople style basis sets, designation of basis set size –Dunnings correlation consistent basis sets. Relativistic effects - Effective core potential, ECP.


MODULE VI: Specifying the molecule in Cartesian and internal coordinates: Writing the Z-matrix of H₂O, CH₄, ethane, Cyclopentadiene, and benzene with suitable point group. Dummy atoms and Ghost atoms. Influence of point group in computations. Illustration by taking H₂O, and NH₃. Computing the quantities-structure, potential energy surface, and chemical properties such as Mulliken and natural charges. Dipole moments. SCF orbital energies. Koopmann’s theorem and Brillouin theorem.

REFERENCES

AIM: To motivate the students to explore renewable energy research especially solar energy.

OBJECTIVES

- To enable the students to master basic aspects of photoexcited states of molecules
- To make the students understand both theory and experiments related to the science of photochemically active systems.
- To provide an idea of recent researches happening in the area of solar energy conversion

COURSE CONTENT


**MODULE II:** Bimolecular Processes: Fluorescence quenching. Collisional quenching. Stern-Volmer equation. Static quenching Photoinduced electron transfer (PET): Concepts and theories, electron donors and acceptors, quantum yield, efficiencies and lifetimes, intermolecular, intramolecular and supramolecular PET. Fluorescence resonance energy transfer (FRET): Trivial or radiative mechanism; Forster and Dexter type energy transfer. Energy transfer versus electron transfer. Applications of electron transfer and energy transfer.

**MODULE III:** Techniques and Instrumentation: Light sources, filters and monochromators: Incandescent lamps and arc lamps, optical filters, spectrographs and monochromators. Lasers as excitation sources: General principles, Two, three and four level lasers, Solid state lasers (Ruby and Nd/YAG) and gas lasers. Luminescence measurements: Steady-state fluorescence spectroscopy. Luminescence quantum yield measurements, Time-resolved fluorescence
spectroscopy, single photon counting, Detection and kinetics of reactive intermediates, Transient absorption spectroscopy: Microsecond and Nanosecond laser flash photolysis. Picosecond laser flash photolysis.

**MODULE IV**: Application of fluorescence in chemical sensing: Various approaches of fluorescence sensing, Fluorescent pH indicators, Fluorescent molecular sensors based on ion or molecular recognition: Recognition units and topology, recognition based on photoinduced electron transfer (PET), photoinduced charge transfer (PCT), Excimer formation and disappearance and Forster resonance energy transfer (FRET). Fluorescent sensors for Metal ions (based on all above mentioned recognition mechanisms), Fluorescent sensors for anions and neutral molecules.


**REFERENCES**

- Depuy C. H. and Chapman, O. L. “Molecular Reactions and Photochemistry”,
- Kavarnos, G. J. “Fundamentals of Photoinduced Electron Transfer”, VCH publishers
• Valeur, B B. “Molecular Fluorescence: Principles and Applications”, Wiley-VCH Verlag
AIM: To introduce analytical principles and environmental chemistry in a general manner

OBJECTIVES

- To introduce data analysis and error calculations
- To introduce certain instrumental techniques
- To introduce and explain the relevance of environmental chemistry

COURSE CONTENT


MODULE III: Instrumental Analysis – an Introduction - An introduction to chromatographic methods – TLC, LC and GC, Geiger-Muller counter and scintillation counter for radioactive detection, Potentiometric and Conductometric analysis of samples, Introduction to
spectroscopic techniques – UV, FTIR and NMR (only principle and application required), Introduction to AAS and ICPMS, SEM and AFM.

**MODULE IV:** Introduction to Environmental Chemistry - Components of Environment. Earth’s atmosphere, Stratosphere chemistry, Ozone formation and depletion, Protection of ozone layer, Chlorofluorocarbons, Chemistry of photochemical smog, Acid rain, Atmospheric production of nitric acid, sulphuric acid, Rain, snow and fog chemistry, Aerosols, Adverse effects of acid rain, Green house effect. Impact of green house effect on global climate.

**MODULE V:** Air and Water Pollution - Air pollution incidents. Control measures for air pollution. Water pollution, Incidents of water pollution in India – examples – causes, effects and remedial measures, Case studies, Humic material, Metal complexes of ligands of anthropogenic origin, Soaps and detergents. Eutrophication.


**REFERENCES**

- van Loon, G. W. “Environmental Chemistry”, OUP.
- Wilson, C. L. and Wilson, D. W. “Comprehensive Analytical Chemistry”, Vol. IB