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

Semester No.	Course code	Name of the Course	No. of Credits
I	*Core courses*		
	CHE-C-411	Inorganic Chemistry I	3
	CHE-C-412	Organic Chemistry I	3
	CHE-C-413	Physical Chemistry I	3
	CHE-C-414	Inorganic Chemistry Lab I	2
	CHE-C-415	Organic Chemistry Lab I	2
	CHE-C-416	Physical Chemistry Lab I	2
II	*Core courses*		
	CHE-C-421	Inorganic Chemistry II	3
	CHE-C-422	Organic Chemistry II	3
	CHE-C-423	Physical Chemistry II	3
	CHE-C-424	Inorganic Chemistry Lab II	2
	CHE-C-425	Organic Chemistry Lab II	2
	CHE-C-426	Physical Chemistry Lab II	2
III	*Core courses*		
	CHE-C-431	Inorganic Chemistry III	3
	CHE-C-432	Organic Chemistry III	3
	CHE-C-433	Physical Chemistry III	3
	CHE-C-434	Inorganic Chemistry Lab III	2
	CHE-C-435	Organic Chemistry Lab III	2
	CHE-C-436	Physical Chemistry Lab III	2
	Internal Elective courses:		
	CHE-E-437 (i)	Advanced Inorganic Chemistry	3
	CHE-E-437 (ii)	Advanced Organic Chemistry	3
	CHE-E-437 (iii)	Advanced Physical Chemistry	3
IV	*Core courses*		
	CHE-C-441	Analytical Principles and Environment	4
	CHE-C-442	Instrumental Methods	4
	Internal Elective courses:		
	CHE-E-443 (i)	Applied Chemistry	4
	CHE-E-443 (ii)	Chemistry of Nanomaterials	4
	CHE-E-443 (iii)	Electronic Structure Theory and Applications	4
	CHE-E-443 (iv)	Photophysical Processes and Applications	4
	CHE-E-443 (v)	Organic Synthesis	4
	Dissertation		
	CHE-D-444	Dissertation	6
Extra Departmental Electives Offered by the Department			
I	CHE-X-411	Analytical and Environmental Chemistry	2

* 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.

FIRST SEMESTER

SEMESTER: **I**

COURSE CODE: **CHE-C-411**

COURSE TITLE: **INORGANIC CHEMISTRY I**

CREDITS: **3**

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 I: Introduction to Coordination Chemistry: Types of ligands and complexes. Coordination number and geometry: Classification of complexes based on coordination numbers and possible geometries. Isomerism: Structural, geometrical and optical isomerism. Stability of complex ions in aqueous solution: Formation constants. Stepwise and overall formation constants. Factors affecting stability of complexes. Determination of stability constants. Irving William order of stability, Chelate and macrocyclic effects.

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^-, R_3P, and Ar_3P. Nephelauxetic series.

MODULE III: Bioinorganic Chemistry: Essential and trace elements in biological systems, structure and functions of biological membranes, mechanism of ion transport across membranes, sodium pump, ionophores, valinomycin and crown ether complexes of Na^+ and K^+, Photosynthesis-chlorophyll a, PS I and PS II. Z-scheme of photosynthesis. Role of manganese complex in oxygen evolution. Coordination compounds in medicine- Anticancer drugs: Platinum complexes- cisplatin. Various types of interaction of metal complexes with nucleic acids.

MODULE IV: Oxygen carriers and oxygen transport proteins-hemoglobins, myoglobins and hemocyanin, hemerythrins and hemevanadins, Iron-Sulphur proteins. Nature of heme-dioxygen binding. cooperativity in hemoglobin. Iron storage and transport in biological systems-ferritin and transferrin. Redox metalloenzymes-cytochromes, peroxidases and superoxide dismutase and catalases. Nonredox metalloenzymes Carboxypeptidase A and Carbonic anhydrase – structure, function and mechanism of action. Nitrogen Fixation - nitrogenase, vitamin B12 and the vitamin B12 coenzymes.

MODULE V: Acid-Base Chemistry and Chemistry in Non-aqueous Solvents: Relative strength of acids, Pauling rules, Lux-Flood concept, Lewis concept, Measurement of acid base strength systematics of Lewis acid – base interactions steric and solvation effects acid – base anomalies , Pearson's HSAB concept, acid- base strength and hardness and softness, Symbiosis, theoretical basis of hardness and softness, electronegativity and hardness. Chemistry in non-aqueous solvents, reactions in NH_3, liquid SO_2, solvent character, reactions in SO_2, acetic acid, solvent character, reactions in CH_3COOH and some other solvents. Molten salts as non-aqueous solvents, solvent properties, room temperature molten salts, unreactivity of molten salts, solutions of metals.

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

- Banerjea, D. "Coordination Chemistry", 3rd Edn., Asian books, 2009.
- Cotton, F. A. and Wilkinson, G., "Advanced Inorganic Chemistry", 6th Edn, Wiley Interscience, New York, 1999.
- Huheey, J. E. Keiter, E. A. and Keiter, R. L. "Inorganic Chemistry - Principles of Structure and Reactivity", 4th Edn, HarperCollins, New York., 1993.
- Kettle, S. F. A. "Physical Inorganic Chemistry: A Coordination Chemistry approach", Oxford University press, 2000.
- Lewis, E. and Wilkins, R. G. (Eds.), "Modern Coordination Chemistry", Interscience, 1967.
- Lippard, S. J. and Berg, J. M. "Principles of Bioinorganic Chemistry", University Science Books, 1994.

ADDITIONAL REFERENCES

- Atkins, P. W. and Shriver, D. F. “Inorganic Chemistry”, 5th Edn, OUP, 2009.
- Bailar, J. C. "Chemistry of Coordination Compounds", Reinhold, 1956.
- Bertini, I, Gray, H. B., Lippard, S. J. and Valentine, J. S., “Bioinorganic Chemistry”, University science books, 1994.
- Cowan, J. A. “Inorganic Biochemistry - An Introduction”, 2nd Edn.,Wiley-VCH, 1997.
- Emeleus, H. J and Sharpe, A. G. “Modern Aspects of Inorganic Chemistry”, 4th Edn., ELBS, 1973.
- Figgis, B. N and Hitchman, M. A. “Ligand Field Theory and its Applications,” Wiley-India, 2010.
- Hay, R.W. Bio Inorganic Chemistry, Ellis Horwood, 1984.
- Holleman, A. F. and Wiberg, E. “Inorganic Chemistry”, Academic press, 2001.
- Lee, J. D. “Concise Inorganic Chemistry,” 4th Edn., Wiley-India, 2008.
- Purcell, K.F and Kotz, J. C. Inorganic Chemistry, Holt-Saunders, 2010.
- Reddy, B. E. Douglas, D. H. McDanial and .Alexander, J. J “Concepts and Models of Inorganic Chemistry”, 3rd Edn, John Wiley, 2001.
- Reddy, K. H. “Bioinorganic Chemistry”, New Age international, 2003

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 II: Stereochemistry of Organic Molecules - Conformational analysis of alkanes and cycloalkanes, Effect of conformation on reactivity of cyclohexane and decalin derivatives. Sawhorse and Newmann projections, Geometrical isomers, E-Z nomenclature, Molecular symmetry and chirality, chiral centres – enantiomers and diastereomers, CIP rules. R and S, threo, erythro nomenclatures, non-carbon chiral centres, Axial and Planar chirality, Atropisomerism, Helicity, stereochemical descriptors for chiral axis and planes, Prostereoisomerism, topicity, Stereoselective and stereospecific reactions, regioselective and regiospecific reactions, calculation of enantiomeric excess and specific rotation, Chiral separation methods, Chiral shift reagents, non-carbon chirality.

MODULE III: Reactions of sp^3 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_Ni 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 sp^2 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 $S_{RN}1$ 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.

MODULE VI: Rearrangement Reactions - Structure, stability and formation of carbocations and carbanions, Classical and non-classical carbocations, Rearrangements including Wagner-Meerwein, Pinacol-Pinacolone, Dienone-Phenol, Beckmann and Benzidine, Baeyer-Villiger oxidation, Demjanov ring expansions, Favorskii and Benzilic acid rearrangements, Ramburg-Buckland reaction, Peterson and Julia olefinations, Structure and synthesis of phosphorus, sulphur and nitrogen ylides, Reactions of ylides including Wittig reaction. Structure, stability and formation of carbenes, nitrenes and benzynes. Bamford-Stevens reaction, Simmon-Smith reaction, Shapiro reaction, Wolff rearrangement, Arndt-Eistert homologation, Hofmann, Curtius, Lossen and Schmidt rearrangements. Addition and insertion reactions of carbenes and nitrenes, Nucleophilic aromatic substitutions and cycloadditions of benzynes.

REFERENCES

- Carey, F. A. and Sundberg, R J. "Advanced Organic Chemistry - Part A: Structure and Mechanisms", 5th Edn, Springer, 2007.
- Lowry, T.H. and Richardson, K. S. "Mechanism and Theory in Organic Chemistry" 3rd Edn, Harper Row, 1987.
- Nasipuri, D. "Stereochemistry of Organic Compounds", 2nd Edn, Wiley Eastern, 1994.
- Smith, M. B. and March, J. "March's Advanced Organic Chemistry", 6th Edn, Wiley. 2007.
- Sykes, P. "A Guidebook to Mechanisms in Organic Chemistry", 6th Edn, Longman, 1986

ADDITIONAL REFERENCES

- Clayden, J., Geeves, N and Warren, S. "Organic Chemistry", OUP.
- Issacs, S. N. "Physical Organic Chemistry", Longman.
- Kalsi, P. S. "Stereochemistry and Reaction Mechanisms", Wiley Eastern, 1993,
- Moody, C. J. and Whitham,W.H. "Reactive Intermediates", 1992, OUP.
- Norman and Coxon, "Organic Synthesis", CRC Press, 3rd En, 1993

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SEMESTER: **I**

COURSE CODE: **CHE-C-413**

COURSE TITLE: **PHYSICAL CHEMISTRY I**

CREDITS: **3**

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 I: Historic evolution of quantum mechanics: The wave nature of sub-atomic particles. The uncertainty principle and its consequences. The postulates of quantum mechanics. Wave functions, well-behavedness, Orthogonality theorem. Orthonormality. Concept of operators: Laplacian, Hamiltonian, linear and Hermitian operators. Angular momentum operators and their properties. Operator algebra, Commutators, Eigen function and eigen values. Expectation value. Time dependent and independent Schrodinger equation. Separation of variables.

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

1. A free particle in 1D. Particle in 1D box of infinite and finite potential wells. Tunnelling. Particle in 3D box. Zero point energy and significance. Applications in conjugated dyes.
2. 1D- Harmonic oscillator. Hermite equation and Hermite polynomials. Recurrence formula. 3D-harmonic oscillator. Oscillator model and Molecular vibrations. Selection rule for vibrational transitions.

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

1. Rigid rotator. Particle on a ring. Separation of variables. Real and Imaginary Wave functions.
2. Non-planar rigid rotator. Legendre and Associated Legende equations and polynomials. Rodrigue's formula. Spherical Harmonics. Polar Diagrams. Salient features. Space quantization.
3. Hydrogen atom. Laguerre and Associated Laguerre equations and corresponding polynomials. Space quantization. Zeeman effect, Uhlenbeck and Goudsmith postulate of spin, Stern Gerlach experiment. Orbitals and Spin orbitals. Radial probability distribution function and graphs. Selection rules for spectral transitions.

MODULE IV: Symmetry and character tables: Symmetry elements and symmetry operations. Point groups. Multiplication of operations. Conditions for a set of elements to form a group. Group multiplication table. Similarity transformation and classification of symmetry operations. Matrix representation of point group. Reducible and irreducible representations. Character of a matrix. Orthogonality theorem. Rules derived from orthogonality theorem (proof not required). Setting up of the character tables of simple groups - C_{2V}, C_{2h}, C_{3V} and C_{4V} on the basis of the rules. Reduction of reducible representations to irreducible representations. Molecular dissymmetry and optical activity. Applications of character tables to spectroscopy. Transition moment operators, vanishing integrals, determination of number of active IR and Raman lines. Application of character table to orbitals. Construction of hybrid orbitals. Construction of Symmetry adapted LCAO

MODULE V: Types of surfaces. Measurements of surface pressure and surface potential. Surfactants and micelles. The gas-solid interface. Types of adsorption. Heat of adsorption. Adsorption isotherms. Gibbs adsorption equation and its verification. Langmuir isotherm. Multilayer adsorption. Freundlich isotherm. BET isotherm. Solid-liquid interface. Influence of surface tension on adsorption. Measurements of surface area of solids. Harkin-Jure method. Entropy and point B methods. Use of Langmuir isotherm and BET method. Eley-Rideal mechanism and the Langmuir-Hinshelwood mechanism

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

- Alexander A. and Johnson P., “Colloid Science,” Oxford University Press, New York, 1996.
- Cotton F. A., "Chemical Applications of Group Theory", Wiley.
- Gregg S. J., “The Surface Chemistry of Solids”, Chapman Hall.
- Jaffe H. and Orchin M., "Symmetry in Chemistry", Wiley.
- Levine I. N., "Quantum Chemistry", 6th Edition, Pearson Education Inc., 2009.
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- Pauling L. and Wilson E. B., “Introduction to Quantum Mechanics”, McGraw Hill., 1935.

ADDITIONAL REFERENCES

- Chandra A. K., "Introduction to Quantum Mechanics", 4^{th} Ed, Tata McGraw-Hill. 1994.
- Hanna M. W., "Quantum Mechanics in Chemistry", 2^{nd} Edition, W. A. Benjamin. Inc. 1969.
- Prasad R. K., “Quantum Chemistry”, 3^{rd} Edition, New Age International, 2006.
- Ramakrishnan V. and Gopinathan M. S., "Group Theory in Chemistry" , Vishal Publications.
- Somorjai A., “Chemistry of Surfaces”, 3^{rd} Edn, Wiley, New York 2005.

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SEMESTER: I

COURSE CODE: CHE-C-414

COURSE TITLE: INORGANIC CHEMISTRY LAB I

CREDITS: 2

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 quatitative estimations using potassium iodate.

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

REFERENCES:

- Skoog, D. A. and West, D. M. "Analytical Chemistry: An Introduction", Saunders.
- Vogel, A. I. "A Text Book of Qualitative Inorganic Analysis", Longman.
- Vogel, A. I. “A Text Book of Quantitative Inorganic Analysis", Longman.

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SEMESTER: I

COURSE CODE: CHE-C-415

COURSE TITLE: ORGANIC CHEMISTRY LAB I

CREDITS: 2

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

- Ahluwalia, V. K. and Aggarwal, R. “Comprehensive Practical Organic Chemistry” Vol 1 & 2, Universities Press.
- Bell, C. E. Taber, D. F. and Clark, A. K. “Organic Chemistry Laboratory”, Thomson.
- Pasto, D. J. Johnson, C. R. and Miller, M. J. “Experiments and Techniques in Organic Chemistry”, Prentice Hall.

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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 I: Distribution law: Partition of iodine, ammonia and aniline between water and organic solvents. Association of benzoic acid. Equilibrium constants of Tri-iodide and copper-ammonium complexes. Enthalpy change for tri-iodide formation.

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 $K_2[HgI_4]$.

MODULE III: Chemical kinetics: Acid hydrolysis of esters. Comparison of strengths of acids. Saponification of esters. Persulphate-iodide second order reaction. Activation energy. Arrhenius parameters. Primary salt effect.

MODULE IV: Thermochemistry: Determination of water equivalent. Heat of neutralization and heat of ionization. Integral and differential heats of solution. Thermometric titrations. Determination of concentrations of strong acids.

MODULE V: Polarimetry: Inversion of cane sugar. Velocity constants for different acid strengths. Comparison of strengths of two acids.

MODULE VI: Adsorption: Verification of Langmuir and Freundlich isotherms for solute adsorption on solids. Estimation of surface area. First order kinetics. Computation of adsorption thermodynamics. Exothermic and endothermic reactions.

REFERENCES

- Daniels, F. and Mathews, J. H. "Experimental Physical Chemistry", Longman.
- Finlay, A. and Kitchener, J. A. "Practical Physical Chemistry", Longman.
- James, A. M. "Practical Physical Chemistry", Churchill.
- Shoemaker, D. P. and Garland, C. W. "Experimental Physical Chemistry", McGraw Hill.
- Willard, H. H. Merritt , L. L. and Dean, J. A. "Instrumental Methods of Analysis", East-West.

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 I: Electronic Spectra of complexes-Term symbols of d^n system. Racah parameters, splitting of terms in weak and strong octahedral and tetrahedral fields. Correlation diagrams for d^n and d^{10-n} ions in octahedral and tetrahedral fields (qualitative approach), *d-d* transition, selection rules for electronic transition-effect of spin orbit coupling and vibronic coupling. Orgel diagrams. Tanabe-Sugano diagrams. Effects of Jahn-Teller distortion and spin-orbit coupling on spectra. Charge transfer spectra. luminescence spectra.

MODULE II: Magnetic properties of metal complexes: Types of magnetism shown by complexes- paramagnetic and diamagnetic complexes, molar susceptibility, Magnetic susceptibility measurements. Gouy method. Spin-only value. Orbital contribution to magnetic moment. Temperature dependence of magnetism- Curie's law, Curie-Weiss law. Temperature Independent Paramagnetism (TIP), Ferromagnetism and antiferromagnetism in complexes. Anomalous magnetic moments. Elucidating the structure of metal complexes (cobalt and nickel complexes) using electronic spectra, IR spectra and magnetic moments.

MODULE III: Reactions of Metal Complexes: Kinetics and mechanism of reactions involving complexes in solution. Inert and labile complexes. Kinetics and mechanism of nucleophilic substitution (Ligand displacement) reactions in square planar complexes. *trans* effect-theory and applications. Kinetics and mechanism of octahedral substitution, Dissociative and associative mechanisms, Ligand field effects on reaction rate. Influence of acid and base on reaction rate. Racemization and isomerization. Redox reactions in complexes: Electron transfer and electron exchange reactions. Theories of Electron transfer reactions-outer sphere mechanism-Marcus theory, inner sphere mechanism, electron transfer in metalloproteins.

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.

MODULE V: Organometallic Compounds-Synthesis, Structure and Bonding: Compounds with transition metal to carbon bonds, classification of ligands, eighteen electron rule. Organometallic compounds with linear pi donor ligands-olefins, acetylenes, dienes and allyl complexes-synthesis, structure and bonding. Complexes with cyclic pi donors-metallocenes and cyclic arene complexes structure and bonding. Carbene and carbyne complexes. Preparation, properties, structure and bonding of simple mono and binuclear metal carbonyls, metal nitrosyls, metal cyanides and dinitrogen complexes. Polynuclear metal carbonyls with and without bridging.

MODULE VI: Reactions of Organometallic Compounds: Substitution reactions-nucleophilic ligand substitution, nucleophilic and electrophilic attack on coordinated ligands. Addition and elimination reactions-1,2 additions to double bonds, carbonylation and decarbonylation, oxidative addition and reductive elimination, insertion (migration) and elimination reactions. Catalysis by organometallic compounds: Homogeneous and heterogeneous organometallic catalysis-alkene hydrogenation using Wilkinson catalyst. Reactions of carbon monoxide and hydrogen-the water gas shift reaction, the Fischer-Tropsch reaction(synthesis of gasoline). Hydroformylation of olefins using cobalt or rhodium catalyst. Carbonylation reactions-Monsanto acetic acid process, carbonylation of butadiene using $Co_2(CO)_8$ catalyst in adipic ester synthesis. Palladium catalysed oxidation of ethylene-the Wacker process.

REFERENCES:

- Banerjea, D. “Coordination Chemistry”, 3rd Edn., Asian books, 2009.
- Cotton, F. A. and Wilkinson, G. “Advanced Inorganic Chemistry”, 6th Edn, Wiley
- Cotton, S. “Lanthanide and Actinide Chemistry”, John Wiley & Sons, 2007.
- Dutta, R. L and Syamal, A. “Elements Of Magnetochemistry”, 2nd Edn., East West press, 1993.
- Huheey, J. E. Keiter, E. A. and Keiter, R. L. “Inorganic Chemistry - Principles of Structure and Reactivity”, 4th Edn, HarperCollins, New York., 1993.
  Interscience, New York, 1999.
- Kettle, S. F. A. "Physical Inorganic Chemistry: A Coordination Chemistry approach", Oxford University press, 2000.
- Mehrotra, R. C. and Singh, A. “Organometallic Chemistry: A Unified Approach”, New age international, 2007.
- Purcell, K. F. Kotz, J. C. ‘Inorganic Chemistry”, Holt-Saunders, 2010.
- Sathyanarayana, D. N. “Electronic Absorption Spectroscopy and Related Techniques”, Universities press, 2001.

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- Bailar, J. C. "Chemistry of Coordination Compounds", Reinhold, 1956.
- Basolo, F. Pearson, R. G. “Mechanisms of Inorganic Reaction”, John Wiley & Sons, 2006.
- Crabtree, R. H. “The Organometallic Chemistry of Transition Metals”, 2Edn, Wiley.
- Drago, R. S. “Physical Methods for Chemists”, 2nd Ed., Saunders College Publishing, 1992.
- Guptha, B. D. Elias, A. J “Basic Organometallic Chemistry”, Universities Press, 2010.
- Holleman, A. F. and Wiberg, E. “Inorganic Chemistry”, Academic.
- Lever, A. B. P. “Inorganic Electronic Spectroscopy”, 2nd Edn., Elsevier, 1984.
- Lewi, E. s and Wilkins, R. G. (Eds.), "Modern Coordination Chemistry", Interscience, 1967.
- Powell, P. “Principles of Organometallic Chemistry”, 2nd Edn., Chapman and Hall, 1988.
- Wilkins, R. G. “Kinetics &Mechanism of Reactions of Transition Metal Complexes”, 2Ed, VCH.

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SEMESTER: **II**

COURSE CODE: **CHE-C-422 (Core)**

COURSE TITLE: **ORGANIC CHEMISTRY II**

CREDITS: **3**

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-Lofler-Freytag and Barton reactions, Use of NBS and tributyl tin hydrides, , Ullmann coupling.

MODULE II: Organic Photochemistry **-** Primary photoprocesses. Jablonski diagram, Photoreactions of C=O systems, enes, eneones, dienes and arenes. Photoisomerisations, Norrish type I and II reactions. Patterno-Buchi and Barton reactions. Di-π-methane and aromatic photo rearrangements. Photochemical remote functionalisation and hydrogen abstraction reactions. Introduction to PET, chemi and bioluminescent reactions. Chemistry of singlet oxygen. Photochemistry in nature. Photosynthesis. Introduction to organic applied photochemistry and femtochemistry, photochromism and thermochromism.

MODULE III: Concerted Reactions - Symmetry properties of MOs. Principle of conservation of orbital symmetry. Pericyclic reactions - theory, mechanism and stereocourse of electrocyclic reactions, cycloaddition reactions and sigmatropic rearrangements, 1,3-dipolar cycloadditions, ene reactions, chelotropic reactions, Sommelet-Hauser, Cope, Claisen and Mislow-Evans rearrangements, thermal eliminations. Woodward-Hoffmann selection rules. secondary orbital interactions in [4+2] cycloadditons, factors affecting rates of cycloaddition reactions.

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, A_2X_3, AB, ABC and AMX type coupling, Coupling constants.. Pascals triangle, first order and non-first order spectra, Karplus curve, Quadrapule 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

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- Coxon, J. M. and Holton, B. "Organic Photochemistry", CUP, 1974.
- Flemming, "Frontier Orbitals and Organic Chemical Reactions", John Wiley, 1998.
- Pavia, D. L. Lampman, G..M. and Kriz, G. S. "Introduction to Spectroscopy" 3rd Edition, Brooks/Cole, 2001.
- Williams, D. H. and Flemming, I. "Spectroscopic Methods in Organic Chemistry", 5th Edition, McGraw Hill. 2011

ADDITIONAL REFERENCES

- Carey, F. A. and Sundberg, R. J. "Advanced Organic Chemistry Part A", 4^{th} Edn. Kluwer, 2007.
- Coyle, J. D. “Photochemistry in Organic Synthesis”, RSC, 1986.
- Kagan, J. “Organic Photochemistry, Principles and Applications”, Paperback, 1993.
- Kalsi, P. S. "Organic Spectroscopy", Wiley Eastern, 2014.
- Kemp, W. "Organic Spectroscopy", Longman. 1991.
- Mc Murry, “Organic Chemistry”, Thomson Brooks/Cole, 1999.
- Norman and Coxon, “Organic Synthesis”, CRC Press, 3^{rd} En, 1993.
- Silverstein, R. M. *et sl*. “Spectrometric Identification of Organic Compounds” 8th Edn, Wiley.
- Wayne, C. E. and Wayne, R. P. “Photochemistry”, OU Primer 39, OUP.

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SEMESTER: **II**

COURSE CODE: **CHE-C-423**

COURSE TITLE: **PHYSICAL CHEMISTRY II**

CREDITS: **3**

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

MODULE I: Many electron atoms- Approximations. Independent particle model. Variational method. Theorem and proof. Variational treatment of hydrogen and helium atom. Secular determinant. Perturbation method – 1^{st} and 2^{nd} order perturbation to energy and wave function. Application to particle in 1-D box of increasing potential, Helium atom. self-consistent field method. Pauli's exclusion principle. Symmetry and antisymmetry wave functions. Slater determinants. Vector atom model. Spin orbit coupling. Spectroscopic Term symbols and spectral lines.

MODULE II: Molecular problems. Born-Oppenheimer approximation. Valence Bond theory (H_2). Molecular Orbital Theory. Ab initio methods. MO theory of hydrogen molecule ion. Electron density distribution and stability of H_2^+ ion. MO theory of H_2 and other homonuclear diatomic molecules. Molecular orbital diagrams, Bond order and stability. MO theory of simple heterogeneous diatomic molecules like HF, LiH, CO and NO. Defects in simple MO and VB theories.

MODULE III: Hartree equations and Hartree-Fock equations for molecular problems. Roothaan modification. Hartree Fock Roothan equations. Electron correlation and relativistic effects, Configuration interaction. Semi empirical MO treatment of planar conjugated molecules. Huckel MO theory and calculation of energy and MO of ethylene, butadiene and allylic anion and cyclic systems – cyclobutadiene and benezene. Calculation of charge distribution, bond order and free valency.

MODULE IV: Spectra of diatomic molecules: Microwave spectroscopy. Rotation of diatomic molecules. Rotational spectrum. Intensity of spectral lines. Calculation of internuclear distance. Nonrigid rotors and centrifugal distortion. Introduction to instrumentation. Infrared spectroscopy: Rotational spectra of polyatomic molecules. Linear and symmetric top molecules. Vibrational spectra of harmonic and anharmonic diatomic molecules. Fundamental and overtones. Determination of force constants. Vibrational rotational couplings. Different branches of spectrum. Symmetry of vibrational-rotation spectrum. Vibrational spectra of polyatomic molecules. Normal modes. Classification of vibrations. Overtones, combination and Fermi resonance. Group frequencies. Introduction to instrumentation and FT IR.

MODULE V: Raman spectra: Scattering of light. Raman scattering. Polarizability and classical theory of Raman spectrum. Quantum theory of Raman spectrum. Rotational and vibrational Raman spectrum. Introduction to instrumentation. Laser Raman spectrum. Raman spectra of polyatomic molecules. Complementarity of Raman and IR spectra.Electronic spectra: Term symbols of molecules. Electronic spectra of diatomic molecules. Vibrational coarse structure and rotational fine structure of electronic spectrum. Franck-Condon principle. Herzberg-Teller vibronic coupling, KHD equation, Fermi Golden rule. Types of electronic transitions. Fortrat diagram. Predissociation. Morse function. Calculation of heat of dissociation. Introduction to instrumentation. Electronic spectra of polyatomic molecules: Electronic transitions and absorption frequencies. Effect of conjugation.

MODULE VI: Resonance spectroscopy: Nuclear spin and interaction with an applied magnetic field. Nuclear resonance. Population of energy levels. ^{1}H NMR spectrum. Chemical shift. Relaxation, Spin-spin coupling, Fine structure; Fourier transform NMR spectroscopy, Nuclear overhauser effect, NMR spectra of other nuclei. Introduction to instrumentation. Electron spin in molecules and its interaction with magnetic field. ESR spectrum. The g factor and its determination. Fine structure and hyperfine structure. Mossbauer spectroscopy: Doppler effect. Chemical shift. Quadrupole effect.

REFERENCES

- Banwell C. N., “Fundamentals of Molecular Spectroscopy", McGraw-Hill.
- Barrow G. M., "Molecular Spectroscopy", McGraw Hill.
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- Daniels F. and Alberty R. A., "Physical Chemistry", Wiley Eastern.
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- Levine I. N., "Quantum Chemistry", 6th Edition, Pearson Education Inc., 2009.
- McQuarrie D. A., "Quantum Chemistry", University Science Books, 1983.
- Pauling L. and Wilson E. B., “Introduction to Quantum Mechanics”, McGraw Hill., 1935.

ADDITIONAL REFERENCES

- Atkins P. W., "Physical Chemistry", OUP.
- Chandra A. K., "Introduction to Quantum Mechanics", 4th Edition, Tata McGraw-Hill. 1994.
- Drago R. S., "Physical Methods in Inorganic Chemistry", Reinhold.
- Hanna M. W., "Quantum Mechanics in Chemistry", 2nd Edition, W. A. Benjamin. Inc. 1969.
- Moelwyn Hughes E. A., "Physical Chemistry", Pergamon.
- Prasad R. K., “Quantum Chemistry”, 3rd Edition, New Age International, 2006.

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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:

- Furman and Welcher, "Standard Methods of Inorganic Analysis", Van Nostrand.
- Kolthoff, I. M. Elving, V. J. and Sandell, “Treatise on Analytical Chemistry”, Interscience.
- Skoog, D. A. and West, D. M. "Analytical Chemistry: An Introduction", Saunders.
- Vogel, I. “A Textbook of Quantitative Inorganic Analysis”, Longman.

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SEMESTER: II

COURSE CODE: CHE-C- 425

COURSE TITLE: ORGANIC CHEMISTRY LAB II

CREDITS: 2

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

- Ahluwalia, V. K. and Aggarwal, R. " Comprehensive Practical Organic Chemistry", Vol 1 & 2, Universities Press.
- Furniss, B. S and others, "Vogel's Textbook of Practical Organic Chemistry", ELBS.
- Silverstein, R. M. *et al.*, "Spectrometric Identification of Organic Compounds", 8th Edn, Wiley.

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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 I: Viscosity: Viscosities of liquids and mixtures of liquids. Verification of Kendall's equation and Jones-Dole equation. Viscosity of polymer solutions. Variation of viscosity with temperature.

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 III: Cryoscopy: Determination of molar freezing points. Depression constant and molecular mass using solid and liquid solvents. Study of dissociation and association of solutes. Atomicity of substances like sulphur.

MODULE IV: Phase equilibria I: CST of phenol-water system. Determination of unknown concentrations of NaCl, acetic and oxalic acid. Construction of phase diagrams of unknown mixtures.

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.

MODULE VI: Transition temperature: Transition temperature of sodium acetate. K_f of sodium acetate. Molecular mass of urea. Transition temperature of sodium thiosulphate.

REFERENCES

- Daniels, F. and Mathews, J. H. "Experimental Physical Chemistry", Longman.
- Finlay, A. and Kitchener, J. A. "Practical Physical Chemistry", Longman.
- James, A. M. "Practical Physical Chemistry", J. A. Churchill.
- Shoemaker, D. P. and Garland, C. W. "Experimental Physical Chemistry", McGraw Hill.
- Yadav, J. B. “Advanced Practical Chemistry”, Goel Publishing House.

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THIRD SEMESTER

SEMESTER : III

COURSE CODE: CHE-C-431

COURSE TITLE: INORGANIC CHEMISTRY III

CREDITS : 3

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 I: Introduction to Solid State: Crystal systems and lattice types. Bravais lattices. Crystal symmetry. Point groups and space groups. Miller indices. Reciprocal lattice concept. Close packed structures: BCC, FCC and HCP. Voids. Coordination number. X-Ray diffraction by crystals: Functions of crystals. Transmission grating and reflection grating. Braggs equation. Diffraction methods. Powder, rotating crystal, oscillation and Weisenberg methods. Indexing and determination of lattice type and unit cell dimensions of cubic crystals. Structure factor. Crystal defects: Point, line and plane defects.

MODULE II: Solid State – Theories and Properties: Binding forces in solids: Ionic bonding and potential energy field. Lattice energy. Born theory and Born-Haber cycle. Molecular, ionic, covalent, metallic and hydrogen bonded crystals. Free electron theory and band theory of solids. Conductors, insulators and semiconductors. Mobility of charge carriers. Hall effect. Electrons and holes. Imperfections and nonstoichiometry (oxides and sulphides). Techniques of introducing imperfections in solids.

MODULE III: Electrical properties of solids: Conductivity of pure metals. Superconductivity. Photoconductivity. Photovoltaic effect. Dielectric properties. Piezoelectricity and ferroelectricity. Magnetic properties of solids: Diamagnetism, paramagnetism, ferromagnetism, ferrimagnetism and antiferromagnetism. Lasers and their applications.

MODULE IV: Structures of Sulphur, Nitrogen, Phosphorus and Silicone Compounds: Sulphur-Nitrogen compounds: Tetrasulphur tetranitride, disulphur dinitride and polythiazyl. S_xN_y 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: Phosphazines. Cyclo and linear phosphazines. Other P-N compounds. Silanes, silicon halides, silicates; Classification and structure, silicones.

MODULE V: Structure of Boron Compounds: Boron hydrides: Reactions of diborane, and its structure and bonding. Polyhedral boranes: Preparation, properties, structure and bonding. The topological approach to boron hydride structure. Styx numbers. Wade's rules. Carboranes: Closo, nido and arachno carboranes. Metalloboranes and metallocarboranes. Organoboron compounds and hydroboration. Boron-nitrogen compounds: Borazine, substituted borazines and boron nitride.

MODULE VI: Other Metal clusters: Factors favouring metal-metal bonds, Dinuclear compounds of Re, Cu and Cr, metal-metal multiple bonding in $(Re_2X_8)^{2-}$, 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:

- Adams, D, M. Inorganic Solids: An Introduction to Concepts in Solid State Structural
- Azaroff, L. V. "Introduction to Solids", McGraw Hill.
- Chakrabarty, D. K. "Solid State Chemistry," New Age Pub., 2010.
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- Cotton, F. A. and Wilkinson, G. "Advanced Inorganic Chemistry", 6th Edn, Wiley
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- Huheey, J. E. Keiter, E. A. and Keiter, R. L. "Inorganic Chemistry - Principles of
  Interscience, New York, 1999.

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- Structure and Reactivity", 4th Edn, HarperCollins, New York., 1993.
- West, A. R. "Solid State Chemistry and its Applications", Wiley.

ADDITIONAL REFERENCES

- Atkins, P. W. and Shriver, D. F. “Inorganic Chemistry”, 5th Edn, OUP, 2009.
- Douglas, B. E. McDanial, D. H. and Alexander, J. J. “Concepts and Models of Inorganic Chemistry”, 3rd Edn, John Wiley, 2001.
- Emeleus, H. J. Sharpe, A. G. “Modern Aspects of Inorganic Chemistry”, 4th Edn., ELBS, 1973.
- Holleman, A. F. and Wiberg, E. “Inorganic Chemistry”, Academic press, 2001.
- Kittel, C. “Introduction to Solid State Physics”, Wiley.
- Lee, J. D. “Concise Inorganic Chemistry,” 4th Edn., Wiley-India, 2008.
- Purcell, K.Fand Kotz, J. C. “Inorganic Chemistry,” Holt-Saunders, 2010.

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SEMESTER : III

COURSE CODE : CHE-C-432 (Core)

COURSE TITLE : ORGANIC CHEMISTRY III

CREDITS : 3

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, PPh_3-CBr_4 reagent

MODULE III: Reagents for oxidation - Oxidations using manganese and chromium reagents, PCC, PDC Collins and Jones reagents, Etard reaction, Use of SeO_2, MnO_2, Ag_2CO_3 and lead tetraacetate, DMSO based reagents - Swern oxidation, Oppenauer oxidation. Oxidation of alkenes - OsO_4, RuO_4, HIO_4, ozone and peracids. Sharpless asymmetric epoxidation, Woodward and Prevost hydroxylations, Dehydrogenation to aromatic compounds. Baeyer-Villiger oxidation, Dakin reaction.

MODULE IV: Reagents for reduction - Catalytic hydrogenation and stereochemistry. Hydrogenation catalysts and their selectivity. Adam's catalyst, Rosenmund reduction, Lindlar catalyst, Wilkinson's catalyst, Homogeneous hydrogenations. Fe, Zn, Na and Li reductions. Dissolving metal reductions – Clemmenson reduction, metal-alcohol reductions, Birch reduction, Hydride transfer reductions – MPV reduction, Reduction using $NaBH_4$, LAH, LAH-$AlCl_3$, DIBAL-H and $NaCNBH_3$. Reductions using borane reagents, hydroboration, Luche reduction, Wolff Kishner and diimide reductions..

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 NH_2 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

- Carruthers, W. “Some Modern Methods of Organic Synthesis”, Cambridge University Press, 2004
- 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
- Warren, S. “Organic Synthesis: The Disconnection Approach”, John Wiley, 2004.

ADDITIONAL REFERENCES

- Harbourne, J. B. “Phytochemical Methods” Chapman Hall.
- House, H. O. "Modern Synthetic Reactions", Benjamin. 1972
- Krishnaswamy, N. K. “The Chemistry of Natural Products,” Universities Press 2010
- Mackie, R. K., Smith, D. M. and Aitken, R. A. “Guidebook to Organic Synthesis”, 3 Edn, Longman.1990
- Mann, J. “Chemical Aspects of Biosynthesis”, Oxford primer 20, OUP.1994
- Norman, R. O. C. and Coxon, A. "Modern Synthetic Reactions", Chapman Hall, 1993
- Simmonds, R. J. "Chemistry of Biomolecules", RSC. 1992
- Smith, M. B. "Organic Synthesis", 2 Edn, McGraw Hill. 1994.

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SEMESTER : III

COURSE CODE: CHE-C-433

COURSE TITLE: PHYSICAL CHEMISTRY III

CREDITS: 3

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

MODULE I: First and second laws of thermodynamics. Thermodynamic criteria for equilibrium and spontaneity. The Clausius inequality, Maxwell relations. The third law of thermodynamics. Need for the third law. Nernst heat theorem. Apparent exceptions to third law. Applications of third law. Thermodynamics of irreversible processes: Simple examples of irreversible processes. General theory of nonequilibrium processes. Entropy production. The phenomenological relations. Onsager reciprocal relations. Application to the theory of diffusion, thermal diffusion, thermoosmosis and thermomolecular pressure difference. Electrokinetic effects. The Glansdorf-Pregogine equation

MODULE II: Statistical thermodynamics: Mechanical description of molecular systems. Thermodynamic property and entropy. Microstates. Canonical and grand canonical ensembles. Equation of state for ideal quantum gases. Maxwell-Boltzman distribution. The partition functions. Partition function for free linear motion, for free motion in a shared space, for linear harmonic vibration. Complex partition functions and partition functions for particles in different force fields. Langevins partition function and its use for the determination of dipole moments. Electrostatic energies. Molecular partition functions. Translational, rotational, vibrational and electronic partition functions. Total partition functions. Partition functions and thermodynamic properties. Heat capacity of gases. Equipartition principle and quantum theory of heat capacity.

MODULE III: Quantum statistics: Bose-Einstein statistics. Examples of particles. Theory of paramagnetism. Bose-Einstein condensation. Liquid helium. Super cooled liquid. Fermi-Dirac statistics. Thermionic emission. Relations between Maxwell-Boltzman, Bose-Einstein and Fermi-Dirac statistics. Heat capacity of solids. The vibrational properties of solids. Einstein theory of heat capacity. The spectrum of normal modes. The Debye theory. The electronic specific heat. Structure of liquids, X-ray diffraction studies, Short range order, radial distribution function, configurational partition function for liquids. Theories of liquids state. Free space and van der Waals theories. Lennard-Jones theory of melting. Specific heats and communal entropy of liquids.

MODULE IV: Order and molecularity of reactions. Time dependency of order. Complex reactions: Reversible, consecutive, concurrent and branching reactions. Free radical and chain reactions. Steady state treatment. Reactions like H_2-Cl_2 and H_2-Br_2. Decomposition of ethane, acetaldehyde and N_2O_5. Rice-Herzfeld mechanism. Unimolecular reaction. Lindemann treatment. Semenoff-Hinshelword mechanism of chain reactions and explosion. Kinetics of fast reactions: Relaxation method. Relaxation spectrometry. Flow method. Shock method. Fast mixing method. Field-jump method. Pulse method. Flash photolysis. Factors influencing reaction rates in solution. Salt effects. Curtin-Hammett equation, kinetic isotope effect.

Theories of reaction rates. Arrhenius equation, Collision theory, potential energy surfaces and reaction coordinate, Transition State theory, comparative study of the theories. Kinetics of reactions in solution. Diffusion controlled reactions. Ionic reactions and effect of ionic strength, Effect of solvents, effects of pressure on velocity of gas reactions.

MODULE V: Catalysis: Mechanism and theories of homogeneous and heterogeneous catalysis. Acid-base catalysis. Skrabal diagram, Bronsted catalysis law, prototropic and protolytic mechanisms, acidity function. Enzyme catalysis. Michaelis-Menton equation, effect of pH and temperature on enzyme catalysis. Mechanism of heterogeneous catalysis- Unimolecular and Bimolecular surface reactions. Langmuir-Hinshelwood mechanism.

Introduction to photochemistry: Laws of photochemistry. Quantum yield. Radiative and non-radiative transitions. Fluorescence and phosphorescence. Intensity and concentration. Fluorescence indicators. Quenching of fluorescence. Chemiluminescence. Explosion reaction. Kinetics of photochemical reaction of H_2 and Cl_2, and H_2 and Br_2. Photopolymerization.

MODULE VI: Ionic activity. Ion-solvent interaction. Strong electrolytes. Ion transport. Debye-Huckel theory of strong electrolytes, Debye-Huckel limiting law. Mean ionic activity coefficient. Debye-Huckel-Onsagar equation and its derivation. Debye-Falkenhagen effect. Wein effect.
Types of electrodes. Electrochemical cells. Liquid junction potential and its determination. Evaluation of thermodynamic properties and activities. Electrical double layer, and its various models. Electrode-electrolyte interface. Electrokinetic phenomena. Current-potential curves. Over potential and its theories. Butler-Volmer equation. Tafel and Nernst equations. Corrosion and methods for prevention. Porbaux diagram and Evans diagram. Introduction to polarography, cyclic voltammetry. Theory and working of Fuel Cells.

REFERENCES

- Moelwyn-Hughes E. A., "Chemical Kinetics and Kinetics of Solution", Academic.
- Panchenkov G. M. and Labadev V. P., "Chemical Kinetics and Catalysis", MIR Publishing.
- Prigoggine I., “An Introduction to Thermodynamics of Irreversible Processes”, Interscience.
- Yenemin E. N., "Fundamentals of Chemical Thermodynamics", MIR Publishers.

ADDITIONAL REFERENCES

- Atkins P. W., “Physical Chemistry”, OUP.
- Daniels F. and Alberty R. A., “Physical Chemistry”, Wiley.
- Maron G. H. and Land J. B., “Fundamentals of Physical Chemistry”, Macmillan.
- Rose J., "Dynamic Physical Chemistry", Issac Pitman.
- Sears F. W., “Introduction to Thermodynamics, Kinetic Theory of Gases and Statistical mechanics”, Addison Wesley.

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SEMESTER : **III**

COURSE CODE : **CHE-C-434**

COURSE TITLE: **INORGANIC CHEMISTRY LAB III**

CREDITS : **2**

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

- Drago, R. S. "Physical Methods in Inorganic Chemistry", Affiliated East-West.
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- Kolthoff, I. M. and Strenger, "Volumetric Analysis", Interscience.
- Kolthoff, I. M., Elving, V. J. and Sandell, "Treatise on Analytical Chemistry", Interscience.
- 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
- Ahluwalia, V. K. and Aggarwal, R. “Comprehensive Practical Organic Chemistry”, Vol 1 & 2, Universities Press.
- Vishnoi, A. K. “Advanced Practical Organic Chemistry” Vikas Publishing, 2009

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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 I: Nuclear and radiation chemistry: Fission products and fission yield. Neutron capture cross section and critical size. Nuclear fusion reactions and their applications. Chemical effects of nuclear transformations. Positron annihilation and autoradiography. Synthesis of transuranic elements such as Neptunium, Plutonium, Curium, Berkelium, Einsteinium, Mendelevium, Nobelium, Lawrencium and elements with atomic numbers 104 to 109. Analytical applications of radioisotopes-radiometric titrations, kinetics of exchange reactions, measurement of physical constants including diffusion constants, Applications of radio isotopes in industry, medicine, autoradiography, radiopharmacology, radiation safety precaution, nuclear waste disposal. Radiation chemistry of water and aqueous solutions. Measurement of radiation doses. Relevance of radiation chemistry in biology, organic compounds and radiation polymerization.

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 III: Inorganic Spectroscopic Methods: Studies of simple inorganic compounds and metal complexes using IR, Raman and NMRSpectroscopy- Metal ligand vibrations, bonding modes of acetate, nitrate, sulphate and perchlorate and metal atoms. Application of IR spectroscopy for the identification of these bonding modes. Far IR spectra. Vibrational spectra of metal carbonyls. CD and ORD of metal complexes. Application of NMR spectroscopy for the structural investigation of diamagnetic metal complexes from chemical shift and spin-spin coupling.

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 V: Inorganic photochemistry: Photochemical laws and kinetics. Photophysical processes. Excited states, ligand field states, charge-transfer states. Fluorescence and phosphorescence. Photochemical reactions-substitution and redox reactions of Cr(III), Ru(II) and Ru(III) complexes. Applications-synthesis and catalysis, chemical actinometry and photochromism. Metal complex sensitizers-electron relay, semiconductor supported metal oxide systems, solar energy conversions; water photolysis, nitrogen fixation and CO_2 reduction. Chlorophyll and light reaction in photosynthesis.

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:

- Arnikar, H. J. “Essentials of Nuclear Chemistry”, Wiley Eastern, 1982.
- Balzani, V and Carassiti, V. “Photochemistry of Coordination Compounds”, Academic Press, 1970.
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- Huheey, J. E. Keiter, E. A. and Keiter, R. L. “Inorganic Chemistry - Principles of Structure and Reactivity”, 4^{th} Edn, HarperCollins, New York., 1993.
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- Porterfield, W. W. “Inorganic Chemistry: A Unified Approach”, Academic Press, 1993.
- Wilkins, R. G. “Kinetics & Mechanism of Reactions of Transition Metal Complexes”, 2^{nd} Edn, VCH.

ADDITIONAL REFERENCES

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- Agarwal, C. V. “Chemistry of Engineering Materials”, 9th Edn., B.S. Pub., 2006.
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- MacGillyvray, L. R and Lukehart, C. M. “Metal Organic framework materials”, Wiley, 2014
- Mehrotra R. C. and Singh, A. “Organometallic Chemistry: A Unified Approach”, New age international, 2007.

  Press, 1994.

- Purcell, K. F and Kotz, J. C. “Inorganic Chemistry”, Holt-Saunders, 2010.
- Roundhill, D. M. “Photochemistry and Photophysics of Metal Complexes”, Plenum

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SEMESTER : III

COURSE CODE : CHE-E-437 (ii)

COURSE TITLE: ADVANCED ORGANIC CHEMISTRY

CREDITS : 3

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
- Io 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 I: Supramolecular Chemistry - Noncovalent interactions: Molecular and chiral recognition, Host-Guest chemistry and inclusion complexes: crown ethers, cryptands, calixarenes, cyclophanes and cyclodextrins, Self-Assembly and Self-Organization, Molecular Aggregates: LB films, lipid membranes, nanotubes, micelles and liquid crystals, Fullerene based supramolecular systems, Dendrimers, Molecular devices: molecular switches and wires, Molecular recognition in biological systems like DNA and proteins.

MODULE II: Green Chemistry - Background, origin and principles of green chemistry. Atom economy and other metrics of greenness. Examples of green processes. Solid supports, Supercritical carbon dioxide, Microwave and sonochemical synthesis. Synthesis using solventless or alternate media conditions: fluorous and ionic liquid media. Green chemistry and sustainable development - pollution control to pollution prevention.

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 IV: Polymer Chemistry - Classes of polymers. Types and mechanisms of polymerization reactions (free-radical, cationic and anionic). Methods of molecular mass and size distribution determination. GPC and Light scattering techniques, Polymer structure and property characterisation. Synthesis of stereoregular polymers. Polymerization techniques. Bulk, Solution, melt, suspension, emulsion and dispersion techniques, Group Transfer, metathesis and ring opening polymerization. Copolymerization. Polymers as supports, reagents and catalysts, Biodegradable polymers, conducting polymers.

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).

MODULE VI: Quantitative analysis of organic functional groups - Analysis of oils and fats. Principle of the analysis of milk and starch based food materials. Analysis and estimation of organic pollutants, Organic trace analysis using spectrophotometry and fluorimetry.

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- Ahluwalia, V. K and Chopra, M. “Medicinal Chemistry”, Ane Books, 2008.
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SEMESTER : **III**

COURSE CODE : **CHE-E-437(iii)**

COURSE TITLE: **ADVANCED PHYSICAL CHEMISTRY**

CREDITS : **3**

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.

Metal complex catalyzed reactions. Hydrogenation. Wacker oxidation. Monsanto acetic acid synthesis. Hydroformylation. Thermal and photochemical Water Gas Shift reactions. Olefin metathesis. Fischer-Tropsch reaction. Mobil process for the conversion of methanol to gasoline hydrocarbons. Ultrafast reaction dynamics. Introduction. Ultrafast lasers. Supersonic beams - pump-probe spectroscopy. Applications.

MODULE II: Corrosion and its Control: Nernst Theory, Standard Electrode Potential, Galvanic Series, Concentration cell, Types of corrosion: Uniform and Galvanic, Erosion, Crevice, Pitting, Exfoliation and Selective leaching, Inter-angular Stress, Waterline, Soil, Microbiological. Theories of corrosion: Acid, Direct Chemical attack, Electrochemical, Corrosion reactions, Factors affecting corrosion, Protective measures against corrosion, Sacrificial anode, and impressed current cathode protection.

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.

MODULE IV: Electrochemical storage cells: Charging and discharging, storage density, energy density. Different types of batteries: (i) Lead Acid (ii) Nickel-Cadmium, (iii) Zinc manganese dioxide. Modern batteries: (i) Zinc-Air (ii) Nickel-Metal Hydride, (iii) Lithium battery. Fuel cells; thermodynamic efficiency, electromotive force of fuel cells: Low temperature fuel cells: Hydrogen–oxygen fuel cells– alkaline and polymeric membrane types. Basics of Microbial fuel cells: construction, electrodes used, electron transfer mechanism.

MODULE V: Advanced Photochemistry: Energy transfer- theories of energy transfer, Photosensitization of organic and inorganic molecules – Singlet oxygen – methods of singlet oxygen generation and detection – chemistry of singlet oxygen – photodynamic therapy of cancer. Photoinduced electron transfer (PET) - concepts and theories. Photochemistry and Photophysics of semiconductors – semiconductor photocatalysis and applications. Artificial solar energy harvesting- photochemical splitting of water, dye sensitized solar cells.

MODULE VI: Computational Chemistry:Empirical, Semi empirical and ab initio methods. Hartree-Fock SCF methods. Basis functions- STO and GTO, primitive and contracted functions. Basis sets. Minimal, split-valence, polarized and diffused, Effective core potential (ECP). Pople style basis sets and examples. Calculating the number of basis functions for a molecular calculation. Molecular properties. Mulliken charges. Dipole moments. Geometry. Molecular orbitals-occupied and virtual. Overlap and overlap population. Specification of molecular geometry in Cartesian coordinates and internal coordinates. Z-matrix of molecules H_2O, NH_3, CH_4, eclipsed and staggered ethane. Dummy atoms and ghost atoms.

REFERENCES

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- Banerjee S. N., "An Introduction to Corrosion Science and Corrosion Inhibition", Oxonian Press P. Ltd., New Delhi, 1985.
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- Sastry V. S., "Corrosion Inhibitors, Principles & Applications", V.S. Sastry, John Wiley & Sons.

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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 I: Conductance: Verification of Onsagar equation. Solubility of sparingly soluble substances. Oswald's dilution law. Basicity of acids. Dissociation constants of acids and bases. Conductometric titrations involving acid-base and precipitation reactions. Equivalent conductance of solutions of strong electrolytes and weak electrolytes.

MODULE II: Potentiometry: Single electrode potentials of hydrogen and glass electrodes. Quinhydrone electrode. Potentiometric titrations involving acid-base, redox and precipitation reactions. pH of buffer solutions. Solubility of AgCl. Determination of dissociation constant.

MODULE III: Polarography: Polarographic estimation of cadmium, zinc and lead. Composition of mixtures.

MODULE IV: Flame photometry: Estimation of Na^+, K^+, Li^+, Ca^{2+} and Mg^{2+}. 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

- Kanetkar Y. P., "Let us C++" 2nd Edition, BPB Publications, Delhi, 2003.
- Vogel A.I., "A Text Book of Quantitative Inorganic Analysis", Longman.
- Willard H. H., Merritt L. L. and Dean J. A., "Instrumental Methods of Analysis", Affiliated East -West.
- Yadav J. B., "Advanced Practical Chemistry", Goel Publishing House.

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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 IV: Modern Organic Synthesis **-** Nef reaction, Kulinkovich reaction, Ritter reaction, Seyferth-Gilbert homologation, Tishchenko reaction, Fritsch-Buttenberg-Wiechell rearrangement, Corey-Fuchs reaction, Noyori reaction. Brook rearrangement. Tebbe olefination. Metal mediated C-C and C-X coupling reactions: Heck, Stille, Suzuki, Suzuki-Miyaura, Negishi-Sonogashira, Nozaki-Hiyama, Buchwald-Hartwig, Ullmann and Glaser coupling reactions. Wohl-Ziegler reaction. Introduction to MCR, Ugi and Passerini reactions, Click reactions, olefin metathesis.

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 $LiAlH_4$, Chiral Catalysts – CBS Catalyst.

MODULE VI: Reagents – Use of DDQ, iodobenzene diacetate, CAN, manganese acetate, $FeCl_3$, NMO, Dess Martin periodinane, SmI_2, N-heterocyclic carbenes, Na tetracarbonyl ferrate, benzenetricarbonyl chromium: TEMED, TEMPO, TMS, $CBr_4 + Ph_3P$

REFERENCES

- Clayden, J., Geeves, N and Warren, S. "Organic Chemistry", OUP.
- Gilchrist, T. L. "Heterocyclic Chemistry." Pearson, Third Edn., 2005.
- Joule J. A and Mills K. "Heterocyclic Chemistry", 4th Edition, UK, Blackwell Science, 2000.
- Norman, R. O. C. "Principles of Organic Synthesis", Chapman and Hall, 2nd Edition, 1995.
- Taber, D **"**Organic Synthesis – State of the Art 2003-2005".
- Warren,S. "Organic Synthesis – The Disconnection Approach", John Wiley and Sons, 2004

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SEMESTER : IV
COURSE CODE : CHE-C- 441 (Core)
COURSE TITLE: ANALYTICAL PRINCIPLES AND ENVIRONMENT
CREDITS : 4

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 I: Data Analysis - Accuracy and precision. Evaluation of analytical data, The mean and median. Standard deviation, variance and coefficient of variation. Classification of errors. Minimization of errors. Significant figures and computations. Statistical methods in analysis. Students T test, Rejection of suspected value, Q test.

MODULE II: Classification of reactions in volumetry (titrimetry)-acidimetry and alkalimetry, redox titrations and complexometric titrations. Acid-base equilibria in water. Ionization constant - role of solvent. Classification of solvents. Leveling and differentiating solvents. Acid-base equilibria in nonaqueous solvents. Buffers. Titration curves. Titrations in nonaqueous solvents. Theories of indicators of different types. Solubility products. Supersaturation and precipitate formation. Mechanism of precipitate formation. Aging of precipitates. Precipitation from homogeneous solutions. Purity of precipitate. Coprecipitation and postprecipitation. Contamination of precipitates. Washing of precipitate. Ignition of precipitate. Fractional precipitate. Organic reagents used in gravimetry - oxine, dimethylglyoxime and cupferron.

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-SO_2, NO_2, NH_3, O_3, and SPM. Principle of the analysis of milk and starch based food materials, Analysis of drugs, oils and fats.

MODULE V: Introduction to Environmental Chemistry **-** Components of Environment. Environment and development. Earth's atmosphere, Stratosphere chemistry, Processes for catalytic decomposition for ozone, Chlorofluorocarbons, Protection of ozone layer, Chemistry of photochemical smog, Composition of 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. Air pollution incidents. Control measures for air pollution.

MODULE VI: Hydrosphere and Solid Waste Management - Physical and chemical properties of water, Organic matter in water, Humic material, Metal complexes of ligands of anthropogenic origin, Water pollutants. Soaps and detergents. Eutrophication. Oil pollution. Heavy metals. Industrial waste water treatment: Solid wastes from mining and metal production, Organic wastes, Mixed urban wastes, Solid waste management, Pollutants in soil. Radioactive pollutants. Pollutants from industries and agriculture. Chemical toxicology. Biochemical effects of pesticides and heavy metals.

REFERENCES

- Bailey, R. A. Clark, H. M. Perris, J. P. Krause, S. Strong, R. L. "Chemistry of the Environment", Academic Chemistry, 8th Edn., Saunders College Pub., 2007.
- De, A. K. "Environmental Chemistry", John Wiley.
- Dick, J. G. "Analytical Chemistry", McGraw Hill.
- Harris, D. C "Quantitative Chemical Analysis", 8th Edition, 2010, WH Freeman and Company, New York.
- Jeffery, G.H. Bassett, J. Mendham, J. Denney, R. C. Vogel's Text Book of
- Manjooran, K. B. "Modern Engineering Chemistry", Kannatheri Publications, Kochi.
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- Wilson, C. L. and Wilson, D. W. "Comprehensive Analytical Chemistry", Vol. IB.

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SEMESTER : **IV**
COURSE CODE : **CHE-C- 442 (Core)**
COURSE TITLE: **INSTRUMENTAL METHODS**
CREDITS : **4**

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 I: Introduction to Instrumental Methods Electrical and nonelectrical data domains-transducers and sensors, detectors, examples for piezoelectric, pyroelectric, photoelectric, pneumatic and thermal transducers. Criteria for selecting instrumental methods - precision, sensitivity, selectivity, and detection limits. Signals and noise: sources of noise, S/N ratio, methods of enhancing S/N ratio– hardware and software methods.Electronics: transistors, FET, MOSFET, ICs, OPAMs. Application of OPAM inamplification and measurement of transducer signals.

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 III: Radiation Analysis Methods Measurement of radioactivity. Detection counters. Ionization chamber, Cloud chamber, Bubble chamber, Proportional counter, Geiger counter, Scintillation counters, Neutron activation analysis. Isotope dilution methods. Introduction to Positron emission Tomography, Working of nuclear reactors.

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.

MODULE VI: Fundamentals of Spectrochemical Methods**,** Spectrophotometers - Sources of Light , Lamp and lasers, Monochromators, Detectors- PMT, Photodiode array, Charge coupled device, Infrared Detectors, Optical Sensors, Dealing with noise- Signal Averaging, Types of Noises, Fourier transformation in infrared Spectroscopy and NMR, Michelson interferometer, Instrumentation of UV-Vis, IR, Fluorescence Spectrometer **Atomic Spectrometry-** Atomization, Flames, furnaces and plasmas, Temperature Effects on Atomic spectroscopy, Inductively coupled Plasmas, Hollow Cathode Lamp, Interferences, Isobaric Interference Back ground Correction techniques, Mass Spectrometry, Ionization Methods Types of Mass Spectrometer, Quadrupole Spectrometer, Time of Flight, Orbitrap, Ion Mobility Mass Spectrometer . Chromatography – Mass Spectrometry – Hyphenated methods, Introduction to ICPMS, XPS.

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- Harris, D. C "Quantitative Chemical Analysis", 8th Edition, 2010, WH Freeman and Company, New York.
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SEMESTER : IV
COURSE CODE : CHE-D- 444
COURSE TITLE: DISSERTATION
CREDITS : 6

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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SEMESTER: **IV**
COURSE CODE: **CHE-E-443 (i)**
COURSE TITLE: **APPLIED CHEMISTRY**
CREDITS: **4**

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

MODULE I: Petroleum, Fuels & Combustion, Lubricants - Petroleum: Petroleum, cracking, Synthetic petrol, Refining of gasoline, Reforming, Chemical structure of fuel and knocking. Octane Rating of fuels, Cetane Rating, Diesel engine fuel, Kerosene, LPG as a fuel.
Fuels & Combustion: Classification, Calorific value, Types, Determination by Bomb calorimeter, Dulong's Formula, Analysis of Coal, Proximate and Ultimate analysis, Fuel gas analysis, Significance, Numericals, Carbonization of Coal, Manufacture of metallurgical coke by Otto Hoffman's by product oven, Combustion calculations.
Lubricants: Functions of lubricant, Mechanism of lubrication, Fluid or Hydrodynamic Lubrication, Thin film or Boundary lubrication & Extreme pressure lubrication. Lubricants for Extreme ambient conditions and for special applications. Properties of lubricants and tests.

MODULE II: Corrosion and Protective Coatings - Corrosion and its Control: Nernst Theory, Standard Electrode Potential, Galvanic Series, Concentration cell, Types of corrosion: Uniform and Galvanic, Erosion, Crevice, Pitting, Exfoliation and Selective leaching, Inter-angular Stress, Waterline, Soil, Microbiological. Theories of corrosion: Acid, Direct Chemical attack, Electrochemical, Corrosion reactions, Factors affecting corrosion, Protective measures against corrosion, Sacrificial anode, and impressed current cathode protection.
Protective Coatings: Paints: Constituents, functions & mechanism of drying. Varnishes and Lacquers; surface preparation for metallic coatings, electroplating (gold) and electroless plating (Nickel), anodizing, phosphate coating, powder coating & antifouling coating.

MODULE III: Applied Inorganic Chemistry - Introduction to chemical industry: Flow sheet preparation. Principles of process selection and operation selection. Basic raw materials and routes to major inorganic products. Flow sheets and engineering aspects of the manufacture of sulfuric acid, ammonia, urea, glass. Refractories: Definition, Classification with examples; Criteria of a good refractory material; Causes for the failure of a Refractory Material. Flow sheet and engineering aspect of the manufacture of Refractories.

MODULE IV: Portland Cement: Manufacture of cement, Dry and Wet process, Flow sheet and engineering aspect of the manufacture of Portland cement, Important process parameters for manufacturing a good cement clinker. Characteristics of the constitutional compounds of cement. Additives for cement, Properties, General composition, testing of cement, Chemical & physical requirement.

MODULE V: Applied Organic Chemistry - Raw materials and routes to major organic products. Flow sheets and engineering aspects of the manufacture of important products such as nitrobenzene, vinyl chloride, soaps, detergents and hydrogenation of oils.
Pharmaceuticals: manufacturing process of aspirin, vitamin A and paracetamol.
Pesticides: manufacture of BHC, DDT, Carbaryl and Malathion. Manufacture of dyes.
Cosmetics: Talcum Powder, Tooth pastes, Shampoos, Nail Polish, Perfumes, soaps, and detergents - General formulations and preparation - possible hazards of cosmetics use.
Adulterants: Adulterants in milk, ghee, oil, coffee powder, tea, asafoetida, chilli powder, pulses and turmeric powder - identification. Color chemicals used in food-soft drinks and its health hazards.

MODULE VI: Polymer Chemistry - Polymers: Types of Polymerization. Thermoplastics & thermosetting polymers. Preparation, properties and applications of the Polyethylene, Teflon, PVC, Nylon, Phenol formaldehyde & Urea Formaldehyde. Silicone resins, silicone fluids, silicone greases. Polyurethanes, foamed or cellular plastics. Elastomers: Natural rubber, Vulcanization of rubber & Synthetic rubber.

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SEMESTER : **IV**
COURSE CODE : **CHE-E-443 (ii)**
COURSE TITLE : **CHEMISTRY OF NANOMATERIALS**
CREDITS : **4**

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 I: Properties of Nanomaterials **-** Difference in behavior between bulk and nanomaterials, Size and dimensionality effects, Quantum size effect. Nanoscale confinement of electronic interactions, Quantum confined materials, Novel optical and magnetic properties of nanomaterials. Quantum dots and its fluorescence, Metal nanoparticles, Surface Plasmon Resonance, Magnetic nanoparticles, Superparamagnetism in nanoparticles. Environmental Issues of nanomaterials.

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,

MODULE V: Characterization of Nanomaterials- Optical Characterization, UV Visible Spectroscopy, Spectrofluorometry, Dynamic light scattering method, X –ray Diffraction and Scherrer Method, Surface Plasmon resonance spectroscopy. Structural Characterization using AFM, STM, SEM, HRTEM and XPS.

MODULE VI: Applications of Nanomaterials - Nanophotonic devices, Nanophotonics for biotechnology and nanomedicine, Hyperthermia with Magnetic nanoparticles, Drug delivery, Nanoparticle for optical diagnosis and targeted therapy, Bio-imaging with quantum dots, Introduction to Nanosensors, FRET, SERS, Graphene–Supercapacitors, Biocompatibility and toxicity of nanoparticles.

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SEMESTER : **IV**

COURSE CODE : **CHE-E-443 (iii)**

COURSE TITLE: **ELECTRONIC STRUCTURE THEORY AND APPLICATIONS**

CREDITS : **4**

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 I: Molecular dynamics: Brief description of computational methods: *ab initio*, semi empirical, and empirical methods. Molecular mechanics. Potential energy functions. Force fields. Geometry minimization, Molecular dynamics. Periodic boundary conditions, Propagation of Newton's equation using Verlet, Velocity verlet and Leap-Frog algorithm.

MODULE II: *Ab initio* Methods: Approximations. Hartree Fock method. Self consistent field. Slater determinants. Roothan approximation. Restricted Hartree Fock (RHF), Restricted open HF (ROHF), and Unrestricted HF (UHF) methods. Semi empirical treatments: Extended Hückel theory. Introduction to CNDO, INDO, NDDO. Applications. Computing the matrix elements. Slater's rules for matrix elements. Convergence. Optimization.

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 IV: Post HF methods- Exchange and Correlation energy. Static and dynamic electron correlation, Avoided crossings and configuration mixing. Configuration Interaction (CI). Couple cluster, Multi-Configuration and Complete active space SCF (MCSCF, and CASSCF), Moller-Plesset Perturbation methods (MP_n). Pros and Cons of these methods.

MODULE V: Density Functional Theory: Development of density function theory (DFT). Density matrices. Thomas-Fermi model. Hohenberg-Kohn existence and variational theorems. Chemical potential. Kohn-Sham self consistent field method. Exchange correlation functionals. Local density approximation (LDA), density Gradient corrections (GGA). Hybrid and meta–GGA functionals. Advantages and applications of DFT.

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MODULE VI: Specifying the molecule in Cartesian and internal coordinates: Writing the Z-matrix of H_2O, CH_4, ethane, Cyclopentadiene, and benzene with suitable point group. Dummy atoms and Ghost atoms. Influence of point group in computations. Illustration by taking H_2O, and NH_3. 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.

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SEMESTER : **IV**

COURSE CODE : **CHE-E-443 (iv)**

COURSE TITLE: **PHOTOPHYSICAL PROCESSES AND APPLICATIONS**

CREDITS : **4**

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 I: Photophysical Properties of the Electronically Excited Molecules: Basic principles of photochemistry: Absorption of radiation-Beer Lambert's law. Electronic transitions. Frank Condon principle. Jablonski diagrams. Nonradiative transitions. Internal conversion and inter system crossing. Radiative transitions: Fluorescence emission, triplet states and phosphorescence. Absorption complexes. Charge transfer absorption. Excimers. Exciplexes. Delayed fluorescence. Chemiluminescence.

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.

MODULE V: Novel Fluorophores: Semiconductor Nanoparticles: Spectral properties of quantum dots, Labeling cells with quantum dots, Quatum dots and Resonance Energy Transfer (RET), Lanthanides: RET with lanthanides, Lanthanide nanoparticles, Near-infrared emitting lanthanides, Long-lifetime metal–ligand complexes: Introduction to metal–ligand probes, Spectral properties of MLC probes, Metal-ligand complex sensors, Aggregation induced emissive (AIE) fluorophores: Mechanism of AIE and applications.

MODULE VI: Solar Energy Conversion:Natural photosynthetic system: Light dependant reactions, photosynthetic reaction centre, Z-scheme of photosynthesis. Artificial photosynthesis, conversion of solar energy to chemical and other forms of energies. Solar water splitting. Photocatalytic hydrogen production, Photocatalytic carbon dioxide reduction. Photovoltaic cells: Polymer solar cells and dye sensitized solar cells. Photo-biochemical energy production.

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SEMESTER: I

COURSE CODE: CHE-X-411

COURSE TITLE: ANALYTICAL AND ENVIRONMENTAL CHEMISTRY

CREDITS: 2

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

OBJECTIVES

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

COURSE CONTENT

MODULE I: Data Analysis - Accuracy and precision. Evaluation of analytical data, The mean and median. Standard deviation, variance and coefficient of variation. Classification of errors. Minimization of errors. Significant figures and computations. Statistical methods in analysis. Students T test, Rejection of suspected value, Q test.

MODULE II: Volumetric Analysis and Precipitation Methods - Classification of reactions in volumetry (titrimetry). Acid-base equilibria in water. Buffers. Titration curves. Theories of indicators. Theory of complexometric titrations and applications, Solubility product. Common ion effect. Super saturation and precipitate formation. Precipitation from homogeneous solutions. The purity of precipitate. Co-precipitation and post precipitation. Contamination of precipitates. Washing of precipitate. Ignition of precipitate. Organic reagents used in gravimetry.

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.

MODULE VI: Solid Waste Management - Heavy metals. Industrial waste water treatment: Solid wastes from mining and metal production, Organic wastes, Mixed urban wastes, Solid waste management, Pollutants in soil. Radioactive pollutants. Pollutants from industries and agriculture. Chemical toxicology. Biochemical effects of pesticides and heavy metals.

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