DEFENCE INSTITUTE OF ADVANCED TECHNOLOGY (DU)

DEPARTMENT OF APPLIED CHEMISTRY

M.Sc. in Applied Chemistry

(Effective from Acad. Year July 2024)

SEMESTER I					
No	**Course Code**	**Course**	**L**	**T/P**	**Credit**
1	AC 501	Inorganic Chemistry-I	3	1	4
2	AC 502	Organic Chemistry-I	3	1	4
3	AC 503	Physical Chemistry-I	3	1	4
4	AC 504	Analytical Chemistry	3	1	4
5	AC 541	Applied Chemistry Laboratory-I	-	4	2
6	RM-501	Research Methodology	4	-	4
SEMESTER II					
1	AC 505	Inorganic Chemistry-II	3	1	4
2	AC 506	Organic Chemistry –II	3	1	4
3	AC 507	Physical Chemistry-II	3	1	4
4	AC 508	Polymer Chemistry	3	1	4
5	AC 542	Applied Chemistry Laboratory-II	-	4	2
6		On Job Training/Internship/Field Project		8	4
SEMESTER III					
1	AC 509	Organometallic Chemistry and Catalysis	3	1	4
2	AC 510	Industrial Chemistry	3	1	4
3	RP-541	Minor Project	3	1	4
4		Elective I	3	1	4
5		Elective II	-	8	4
SEMESTER IV					
1	AC 550	Seminar	-	2	2
2	RP 542	Major Project	-	36	18
		Credits Total			**84**

LIST OF ELECTIVE COURSES

S. No.	**Course Code**	**Course**
1	NT-601	Introduction to Nanoscience and Technology
2	AC-610	Recent Advances in Chemistry
3	AC-511	Molecular Spectroscopy I
4	AC-512	Molecular Spectroscopy II
5	AC-513	Defence Chemistry
6	MS-502	Advanced Characterization Techniques
7	NT-604	Nano-biotechnology
8	ACFT-501	Food Chemistry
9	AC-608	Safety Health and Hazard Management
10		Online courses from NPTEL, MOOC. SWAYAM
11		Open elective from any Department

DETAILED SYLLABUS OF SEMESTER -I

Course Code	Course Name	L – T – P	**Credits**
AC 501	**INORGANIC CHEMISTRY-I**	4-0-0	**4**

Course Objectives:
CO 1: To develop an insight into the basic knowledge of inorganic chemistry
CO 2: To understand chemical bonding, coordination compounds, f-block elements and their theories
CO 3: To apply the knowledge and understanding in the areas of chemical bonding, coordination compounds and f-block elements for solving existing challenges faced in various chemical and industrial area

Course Contents

UNIT I: MAIN GROUP ELEMENTS

Hydrides, halides, oxides, oxoacids, nitrides, chalcogenides – shapes and reactivity. Structure and bonding of boranes, carboranes, silicones, silicates, boron nitride, borazines and phosphazenes. Allotropes of carbon, phosphorous and sulphur. Industrial synthesis of compounds of main group elements. Chemistry of noble gases, pseudo-halogens, and interhalogen compounds. Acid-base concepts and principles

UNIT II: TRANSITION ELEMENTS

Coordination chemistry – structure and isomerism, theories of bonding. Energy level diagrams in various crystal fields, CFSE, applications of CFT. Electronic spectra of transition metal complexes: spectroscopic term symbols, selection rules, nephelauxetic effect and Racah parameter, charge-transfer spectra. Magnetic properties of transition metal complexes. Metal-metal multiple bonds

UNIT III: LANTHANIDES AND ACTINIDES

Recovery, Periodic properties, spectra and magnetic properties.

UNIT IV APPLICATION OF INORGANIC CHEMISTRY IN INDUSTRY

Manufacture of inorganic products on a large scale such as the heavy inorganics (chloralkalis, sulfuric acid, sulfates) and fertilizers (potassium, nitrogen, and phosphorus products)

Course Outcomes

After completing this course, the students will be able to:
CO1: To understand structure and bonding of main group elements,
CO2: Students can familiarize with transition metals and their applications
CO3: To understand the basic properties of rare earth elements
CO4: Use of inorganic chemistry knowledge for application in Industry **(heavy inorganics and fertilizers)**
CO5: Overall students can solve the problems related to Inorganic chemistry

Text Books

1. Concise Inorganic Chemistry - J. D. Lee. Wiley India
2. Inorganic Chemistry -Meissler & Tarr, Pearson New International
3. Mechanism of Inorganic Reactions – Fred Basolo, Ralph G. Pearson

Reference Books
Inorganic Chemistry: Principles of Structure and Reactivity – James E. Huheey

Course Code	Course Name	L – T – P	**Credits**
AC 502	**ORGANIC CHEMISTRY-I**	4-0-0	**4**

Course Objectives:
CO 1: To develop an insight the basic knowledge of organic chemistry
CO 2: To understand structure and reactivity, aromatic nucleophilic substution, stereochemistry of compounds
CO 3: To apply the knowledge and understanding in the areas of structure and reactivity, aromatic nucleophilic substution, stereochemistry of organic compounds for solving existing challenges faced in various chemical and industrial areas

Course Contents

UNIT I: STEREOCHEMISTRY

Chirality and symmetry of organic molecules with or without chiral centres and determination of their absolute configurations. Relative stereochemistry in compounds having more than one stereogenic centre. Homotopic, enantiotopic and diastereotopic atoms, groups and faces. Stereoselective and stereospecific synthesis. Conformational analysis of acyclic and cyclic compounds. Geometrical isomerism and optical isomerism. Configurational and conformational effects, atrop isomerism, and neighbouring group participation on reactivity and selectivity/specificity.

UNIT II: REACTION MECHANISMS

Basic mechanistic concepts – kinetic versus thermodynamic control, Hammond’s postulate and Curtin-Hammett principle. Methods of determining reaction mechanisms through kinetics, identification of products, intermediates and isotopic labelling. Linear free-energy relationship – Hammett and Taft equations. Nucleophilic and electrophilic substitution reactions (both aromatic and aliphatic). Addition reactions to carbon-carbon and carbon-heteroatom (N and O) multiple bonds. Elimination reactions. Reactive intermediates – carbocations, carbanions, carbenes, nitrenes, arynes and free radicals. Molecular rearrangements.

UNIT III: ORGANIC SYNTHESIS

Synthesis, reactions, mechanisms and selectivity involving the following classes of compounds – alkenes, alkynes, arenes, alcohols, phenols, aldehydes, ketones, carboxylic acids, esters, nitriles, halides, nitro compounds, amines and amides. Concepts of multistep synthesis – retrosynthetic analysis, strategic disconnections, synthons and synthetic equivalents. Selectivity in organic synthesis – chemo-, regio- and stereoselectivity. Protection and deprotection of functional groups. Concepts of asymmetric synthesis – resolution (including enzymatic), desymmetrization and use of chiral auxiliaries, organo catalysis. Carbon carbon and carbon-heteroatom bond forming reactions through enolates (including boron enolates), enamines and silyl enol ethers. Stereoselective addition to C=O groups (Cram, Prelog and Felkin-Anh models).

Course Outcomes

After completing this course, the students will be able to:

CO 1. To understand the detailed aspects of Stereochemistry including optical and geometrical isomerism.

CO 2. To gain knowledge on methods of determination of reaction mechanism, various reaction intermediates

CO 3: Design and conceptualization of organic synthesis with several examples

Text Books

1. Stereochemistry Conformation and Mechanism **-**P.S. Kalsi
2. Stereochemistry of Organic Compounds **-** E. L. Eliel
3. A Guidebook to Mechanism in Organic Chemistry – Peter Sykes
4. Modern Methods of Organic Synthesis – William Carruthers, Iain Coldham
5. Organic Synthesis the disconnection approach – Stuart Warren
6. Advanced organic Chemistry: Jerry March, Wiley &Sons

Reference Books: Organic Chemistry **-**Clayden, Greeves, Warren and Wothers

Course Code	Course Name	L – T – P	**Credits**
AC 503	**PHYSICAL CHEMISTRY-I**	4-0-0	**4**

Course Objectives:
CO 1: The learners should be able to apply principles and laws of equilibrium thermodynamics to multicomponent systems. In addition, they should be able to use spectroscopic data to calculate thermodynamic properties of ideal gases, real gases, solids and metals using the principles and techniques of statistical thermodynamics.

Course Contents

UNIT I: THERMODYNAMICS

Brief description of the laws of thermodynamics, Concepts of Entropy and Residual Entropy, Free energy and its Temperature dependence, Thermodynamic Equilibria and Free Energy Functions, Physical Equilibria Involving Phase Transitions, Thermodynamic Maxwell Relations, Statistical Thermodynamics

UNIT II: EQUILIBRIUM THERMODYNAMICS

Partial molar quantities, Determinations of the partial molar quantities, Chemical potential and other thermodynamic functions, Variation of chemical potential with temperature and pressure, Chemical potential for Ideal gas mixture, Thermodynamic Functions of Mixing, Concepts of Fugacity and its determination, non-ideal systems: Excess functions for non-ideal solutions. Gibbs Duhem Margules equation and its applications.

UNIT III: NON-EQUILIBRIUM THERMODYNAMICS

Thermodynamic criteria for non-equilibrium states, Basic Postulates and Methodology, Onsager's Theory, Phenomenological Laws and Equations, Transformations of the generalized fluxes and forces, Microscopic Reversibility and Onsager's Reciprocal Relations, Entropy Production and entropy flow, Theorem of Minimum Entropy Production, Chemical Reactions, Coupled Reactions and Electro-kinetic Phenomena.

UNIT IV: CHEMICAL EQUILIBRIUM

Ideal and Non-ideal solutions, Raoult's Law and Henry's Law, Chemical equilibria. Dependence of equilibrium constant on temperature and pressure. Ionic mobility and conductivity. Debye-Hückel limiting law. Debye-Hückel-Onsager equation. Standard electrode potentials and electrochemical cells. Nernst Equation and its application, relationship between Electrode potential and thermodynamic quantities, Potentiometric and conductometric titrations. Phase rule. Clausius- Clapeyron equation. Phase diagram of one component systems: CO2, H2O, S; two component systems: liquid- vapour, liquid-liquid and solid-liquid systems. Fractional distillation. Azeotropes and eutectics.

Course Outcomes
After completing this course, the students will be able to: **CO1: Understanding of basic chemical thermodynamics** **CO2: To familiarize equilibrium and non-equilibrium thermodynamics** **CO3: To understand and application of various laws of thermodynamics**
Text Books
1. Elements of Chemical thermodynamics – Leonard Nash, Dover Publications 2. Chemical Thermodynamics–Peter A. Rock 3. A text book of Physical Chemistry (Vol-V) – K. L. Kapoor
Reference Books
Fundamentals of Molecular Spectroscopy – Colin N. Banwell

Course Code	Course Name	L – T – P	**Credits**
AC 504	**ANALYTICAL CHEMISTRY**	4-0-0	**4**

Course Objectives: Students will gain an idea about the chromatography, different kinds of titrations methods, Spectroscopic instrumental method of analysis

Course Contents

Unit I: Concepts of Analytical Chemistry

Classification of Analytical Methods: An overview of Classical methods, Types of Instrumental methods Selection of an analytical methods and their performance criteria. Concepts of optical methods: Electromagnetic spectrum, transitions, components in optical instruments, sources, description of LASER, wavelength selectors, monochromator functioning, effective band width, detectors and description of diode array type detector. Atomic Absorption Spectrometry: Principle, interferences, use of electro thermal analyser, hydride generator and cold vapour for trace metal analysis.

Unit II: Electro-analytical techniques

Electrochemistry, Nernst equation, Potentiometry, Amperometry, Electrochemical analysis, Standard hydrogen electrode (SHE), Calomel electrode, Ion selective electrodes (ISE), etc.and their applications.

Unit III: Spectrochemical methods

Introduction, electronic spectra and molecular structure, Concepts of optical methods: Electromagnetic spectrum, transitions, components in optical instruments, General instrumentation for for spectrometer, Absorbance and chromophores, Beer-Lambert's Law.

Unit IV: Thermal Analysis

Thermogravimetric analysis (TGA) and its applications to organic, inorganic and polymer material characterization. Differential scanning calorimetry (DSC) and its application.

Unit V: Chromatography

Fundamental of chromatographic separations, retention time, retention volume, distribution ratio, K factor. TLC, High Performance Liquid Chromatography (HPLC) its application to organic compounds. Gas Chromatography (GC) and applications of chromatography.

Course Outcomes

After completing this course, the students will be able to:
CO1:To understand the basic concepts of analytical chemistry
CO2: To understand various types of spectroscopic techniques and their applications
CO3: To thermal analysis
CO4: To understand the detailed aspects of various separation methods (Chromatographic techniques).

Text Books

1. Analytical Chemistry Skoog and Skoog,
2. ElectroAnalytical Methods, Fritz Scholz, Springer
3. Thermal Analysis Techniques and Applications, N.N. Kaushik and Shukla

Reference Books

Analytical Chemistry, Alka Gupta, Pragati Publication

Course Code	Course Name	L – T – P	**Credits**
AC 541	**APPLIED CHEMISTRY LABORATORY-I**	0-0-4	**2**

Course Objectives: students will gain the knowledge of performing experiments including synthesis & characterization and properties

Course Contents

Synthesis, Purification and Analysis of the following Inorganic Preparations:

1. Bis(ethylene-di-ammine) copper (II) sulphate
2. Hexa-ammine nickel (II) chloride/sulphate

Non-Instrumental Experiments: Thermodynamics, Phase Rule and Reaction Kinetics:

1. Determination of heat of solution of benzoic acid by solubility measurements.
2. Determination of heat of solution of salicylic acid by solubility measurements.
3. Determination of equilibrium constant of the reaction KI + I_2+ KI3 by distribution method.

IV. Synthesis of Organic compounds Synthesis, purification and characterization of about ten organic compounds involving one or two stages.

1. m-dinitrobenzene from Nitrobenzene
2. Aromatic acid from ester
3. Benzanilide from aniline
4. p-nitroaniline from Acetanilide
5. Phthalimide from phthalic acid
6. Benzanilide from Benzophenone

Course Outcomes

After completing this course, the students will be able to:
CO1: To perform synthesis, purification and analysis of Organic and Inorganic Compounds
CO2: To study various physic-chemical properties of mixtures

Selected Text Books

1. Elias, A.J., A Collection of Interesting General Chemistry Experiments, Universities Press, (India) Pvt. Ltd., 2002.
2. Roesky, H. W.; Möckel, K., Chemical Curiosities: spectacular experiments and inspired quotes, VCH, 1996. Hand-outs prepared for the laboratory experiments:

collections from various literature sources

3. l.G., Svehla, 'Vogel's Qualitative Inorganic Analysis',6thEdn., Orient Longman New Delhi, l987.
4. V.V., Ramanujam, 'Inorganic Semi-micro Qualitative Analysis', 3rd Edn., National Publishing Company, Madras, l990.
5. A. I. Vogel, Vogel's Text Book of Quantitative Inorganic Analysis, 6th Ed., Pearson Education, 2000.

Reference Books

1. J. D. Woolins, Inorganic Experiments, Wiley-VCH Verlag GmbH and Co., 2003.
   W. G. Palmer, Experiments in Inorganic Chemistry, Cambridge University Press

DETAILED SYLLABUS OF SEMESTER -II

Course Code	Course Name	L – T – P	**Credits**
AC 505	**INORGANIC CHEMISTRY-II**	4-0-0	**4**

Course Objectives: students will gain the knowledge Bioinorganic Chemistry and its biological applications.

Course Contents

UNIT I:. BIO-INORGANIC CHEMISTRY

Occurrence and availability of Inorganic elements in organisms, transport and storage of Inorganic elements, Dose response of an element, biological function of inorganic elements, beneficial and toxic elements, essential and tracemet

Sidrophore, phytosidrophores, ferretin, transferrin, hemosiderine, biomineralization, assembly of advanced materials e.g. calcium phosphate, calcium carbonate, ironbiominerals.

Oxygen transport and storage through hemoglobin and myglobin, Alternative oxygen transport in lower organisms.

Unit II: Photosynthesis: Photochemistry, absorption spectra of photosynthetic pigments, photophosphorylation - energy conversion process Role of Alkali and alkaline earth metals in neuro sensation. Ion Channels, ion pumps, magnesium catalysis of phosphate, ubiquitous regulatory role of calcium.

UNIT III: Biological ligands for metal ions: Macrocycle, nucleobase, nucleotides and nucleic acids, coordination of metals by protein. Heme and nonheme protein, oxygen uptake, structure and function of haemoglobin, myoglobin, hemocyanin, hemotherine Principle involved and role of various metals viz. Zn, Fe, Cu and Co; carboxy peptidase, carbonic anhydrase, Alcohol dehydrogenase, Zinc Fingures, other gene regulatory Zinc proteins, cobalomine, mutase activities of coenzyme B12.

UNIT IV: APPLICATIONS OF BIO-INORGANIC CHEMISTRY

Medicinal therapy; metal deficiency and disease, toxic effect of metals, metals used for diagnosis and chemotherapy, gold compound as Anti-Rheumatic agent. Nitrogen cycle; biological nitrogen fixation, metalloenzyme in biological nitrogen cycle, molybdenum nitrogenase, other nitrogenase model, Nanoparticles for antimicrobial applications

Course Outcomes

After completing this course, the students will be able to:

CO1: The concept of Bioinorganic Chemistry and its biological applications

CO2: To understand photosynthesis and other photochemical reactions

CO3: Role of bioinorganic chemistry in nature

CO4: Important Applications of Bio-inorganic chemistry

Text Books

1. The Organometallic Chemistry of the Transition Metals, by Robert H. Crabtree, Wiley 2014
2. Organo transition Metal Chemistry: From Bonding to Catalysis by John F. Hartwig, University Science Books, 2009
3. Organo transition Metal Chemistry, Anthony F. Hill, Royal Society of Chemistry, 1. Tutorial Chemistry Text, 2002. Chapters 1 to 7.
4. Inorganic Chemistry – Principles of Structure & Reactivity, J E Huheey, Elllen A

Keiter &
Reference Books
5. Richard L Keiter, IV Edition(2005)

Course Code	Course Name	L – T – P	**Credits**
AC 506	**ORGANIC CHEMISTRY-II**	4-0-0	**4**

Course Objectives:
To impart advanced knowledge of reactive intermediates, stereochemistry of organic compounds, pericyclic reactions, heterocyclic compounds and applications in biomolecules

Course Contents

UNIT I: PERICYCLIC REACTIONS AND PHOTOCHEMISTRY

Electrocyclic, cycloaddition and sigma tropic reactions. Orbital correlations – FMO and PMO treatments, Woodward-Hoffmann rule. Photochemistry of alkenes, arenes and carbonyl compounds. Photooxidation and photoreduction. Di-π-methane rearrangement, Barton-McCombie reaction, Norrish type-I and II cleavage reaction.

UNIT II: HETEROCYCLIC COMPOUNDS

Introduction to heterocyclic compounds and their applications, Structure, preparation, properties and reactions of furan, pyrrole, thiophene, pyridine, indole, quinoline and iso quinoline.

UNIT III: BIOMOLECULES

Structure, properties and reactions of mono- and di-saccharides, physicochemical properties of amino acids, chemical synthesis of peptides, chemical structure determination of peptides and proteins, structural features of proteins, nucleic acids, lipids, steroids, terpenoids, carotenoids, and alkaloids.

UNIT IV: ANALYSIS TECHNIQUES IN ORGANIC CHEMISTRY

Applications of UV-visible, IR, NMR and Mass spectrometry in the structural determination of organic molecules.

Course Outcomes

After completing this course, the students will be able to:
CO1: Understanding of Electrocylcic/cycloadditions and sigmatropic reactions
CO2: To understand photo-oxidation and photo reduction and related rearrangements
CO3: To understand heterocylic and their applications in biomolecules and drugs
CO4: To familiarize students in various analysis techniques

Selected Text Books

1. A Guidebook to Mechanism in Organic Chemistry **– Peter Sykes**
2. Organic Chemistry **-Clayden, Greeves, Warren and Wothers**
3. Modern Methods of Organic Synthesis **– William Carruthers, Iain Coldham**
4. Organic Synthesis the disconnection approach **– Stuart Warren**
5. Pericyclic Reactions – R T Morrison, R N Boyd
6.

Reference Books

Organic Photochemistry – James H. Coxon, B. Halton

Course Code	Course Name	L – T – P	**Credits**
AC 507	**PHYSICAL CHEMISTRY-II**	4-0-0	**4**

Course Objectives: To apply the knowledge and understanding in the areas of solid state chemistry, chemical kinetics and surface chemistry for solving existing challenges faced in various chemical and industrial areas also To understand various phenomena of group theory and spectroscopy.

Course Contents

UNIT I: CHEMICAL KINETICS

Elementary, parallel, opposing and consecutive reactions. Steady state approximation. Mechanisms of complex reactions. Unimolecular reactions. Potential energy surfaces and classical, Activated Complex Theory, Potential energy surfaces- attractive and repulsive forces, Chain reactions and oscillatory reactions, Photochemical reactions. Enzyme kinetics: Michaelis-Menten mechanism- single and double intermediates, Enzyme inhibiton- reversibility and products inhibiton, Molecular beams, principle of crossed-molecular beams. Molecular encounters and principle parameters, e.g. Impact parameter, Collision cross-section, Reaction cross section and relation between reaction cross-section and reaction rate (single velocity). Dependence of collisional cross-section on translational energy. Probing the transition state, Dynamics of barrier-less chemical kinetics in solution, dynamics of unimolecular reactions. Luminescence and energy transfer processes, study of kinetics by stopped-flow technique, relaxation method, flash photolysis and magnetic resonance method. Kinetics of solidstate reactions.

UNIT II: SURFACE CHEMISTRY

Surface tension, Capillary action, Pressure difference across curved surface (Laplace equation), Vapour pressure of droplets (Kelvin equation), Gibbs adsorption isotherm, BET adsorption isotherm, Surface films (Electro-kinetic phenomenon), Catalytic activity at surfaces. Catalysis on metal surfaces, Metal oxide surfaces. General characteristics of catalytic reactions, Acid-base catalysis, Enzyme catalysis, Mechanism and kinetics of enzyme-catalysed reactions, Michaelis-Menten equation, Heterogeneous catalysis, Surface reactions, Autocatalysis and Oscillatory reactions. Surface active agents, Classification of Surface active agents, Co-surfactants, Micellization, Microemulsions, Aggregate structures of surfactants, Critical Micellar Concentration, Surfactant packing parameter, Factors affecting the CMC of surfactants, Counter ion binding to micelles, Hydrophobic interaction, Thermodynamics of micellization, Mass action models, Solubilization and Phase diagram of ternary microemulsion system

UNIT III: GROUP THEORY

Symmetry Elements and Symmetry Operations, Point Groups, Representation of Groups, Reducible and Irreducible Representation; Character Tables, Orthogonality Theorem– Its Consequences; Internal coordinates and vibrational modes; symmetry adapted linear combination of atomic orbitals (LCAO-MO);

Course Outcomes

After completing this course, the students will be able to:
CO1: Understanding rate laws based on Chemical Kinetics
CO2: Understanding different aspects of surface chemistry
CO3: To understand various phenomena of group theory and spectroscopy

Text Books

1.Chemical Applications of Group Theory – F. Albert Cotton

2.Fundamentals of Molecular Spectroscopy – Colin N. Banwell

Reference Books

Physical Methods – Russel S. Drago

Course Code	Course Name	L – T – P	**Credits**
AC 508	**POLYMER CHEMISTRY**	4-0-0	**4**

Course Objectives: To understand fundamental concepts and techniques in polymer chemistry including reaction mechanism and commercial applications

Course Contents

UNIT I: FUNDAMENTAL CONCEPTS

Functionality - principle of polymerisation - addition, condensation polymerisation - ring opening polymerisation - classification - production from coal tar and petrochemicals - Techniques of polymerisation - gas polymerisation, - bulk, solution, suspension and emulsion - melt condensation. Mechanism of polymerisation and general characteristics - free radical - cationic, anionic and coordination polymerisation (Ziegler-Natta catalyst) auto acceleration - Kinetic chain length - degree of polymerisation, kinetics of polymerisation (Detailed study) - copolymerisation.

UNIT II: POLYMER CHARACTERISATION

Molecular weight, MWD - Mn, Mw, Mv and Mz - end group analysis - viscometry - osmometry - Light scattering - spectral analysis-Thermal properties – Polymer rheology, Electrical properties, Mechanical and dynamic properties - polymer degradation. Phase transitions of polymers, crystallization and glass transition, mechanism of glass transition, methods of determining Tg.

UNIT III: STUDIES OF INDIVIDUAL POLYMERS

Plastics - polyolefins, polystyrenes, acrylics, polyesters, polyamides, cellulose, polyurethanes, Inorganic polymers, FIR plastics – GR plastics. alkyd resins, epoxy resins - phenolics - Melamine resins - compounding of plastics - rubber - elastomer - vulcanisation, compression mouldings - injection mouldings - lamination. Biopolymers - Biomaterials - medicinal applications of polymers - High temperature and fire-resistant polymers. Polymer concrete - polymer impregnated concrete - conducting polymers - polymeric reagents.

UNIT IV: POLYMER FOR COMMERCIAL APPLICATIONS

Technology of Production, Properties and Applications of Chain growth polymers

Polyethylene such as HDPE, MDPE, LDPE, LLDPE, HMWPE, UHMWPE, EVA, crosslinked PE, chlorinated PE, Polypropylene (PP), Polyisobutylene (PIB)), Acrylics (PMMA & PAN), Poly-vinyles like PVC, PVDC & CPVC, Polystyrene & Co-polymer (HIPS, SBR, SAN & ABS), Poly(vinyl acetate).

Course Outcomes

After completing this course, the students will be able to:
CO1: To understand fundamental concepts and techniques in polymer chemistry
CO2: Methods of characterization of polymers.
CO3: learn various important polymers.
CO4: Familiarize polymers having commercial applications

Text Books

1. P.J. Flory, 'Principles of Polymer Chemistry', Cornell Press, (Recent Edition).
2. Jr. Billmeyer, 'Test Book of Polymer Science', Fred, W. John Wiley & Sons, N. York, l984.
3. Dan Campbell, Richard A. Pethrick, Jim R. White, Polymer Characterization: Physical Techniques, 2nd Edition, CRC Press, 2012.
4. F. Rodrigues, 'Principles of Polymer Systems', M. Elpaw Hill Book Company, 2nd Ed., l982.
5. K.J. Saunders, 'Organic Polymer Chemistry', Chapman & Hall, London, l973.

Reference Books

1. Sabu Thomas & Dominique Durand, Handbook of Biopolymer-Based Materials: From Blends and Composites to Gels and Complex Networks, Wiley – VCH, 2013.

Course Code	Course Name	L – T – P	**Credits**
AC 542	**APPLIED CHEMISTRY LABORATORY - II**	0-0-8	**2**

Course Objectives: To acquire basic knowledge of various instrumental methods of analysis and synthesis with their characterization

Course Contents

1. pH metry / conductometry / potentiometry and precipitation titrations

2. Determination of critical miceller concentration of surfactants.

3. Preparation and TLC demonstration of the purified product and determination of MP and % yields, etc.

   1. Bromobenzene to p-nitro bromobenzene
   2. Nitrobenzene to m-dinitrobromobenzene

3. Benzoin to Benzil
4. Anthracene to Anthraquinone
5. Anthracene-Maleic Anhydride adduct

Course Outcomes

After completing this course, the students will be able to:
CO1: To familiarize various electro-analytical/optical techniques
CO2: Synthesis and characterization of organic compounds

Text Books

Reference Books

1. Elementary Practical Organic Chemistry Part-I small scale preparations, A.L. Vogel (Longman)
2. Laboratory Manual of organic chemistry, B.B. Dey and M.V. Sitaram revised by T.R Govindachari (Allied Publishers Ltd)
3. D.P.Shoemaker, C.W.Garland & J.W.Nibber,,'Experiments in Physical Chemistry', McGraw Hill 5th Edn., 1989.
4. A. I. Vogel, 'Text book of Practical Organic Chemistry',5thEdn. ELBS, London, l989.
5. B.B.Dey and M.V.Sitharaman,'Laboratory Manual of Organic Chemistry' Revised by T.R. Govindachari, Allied Publishers Ltd., New Delhi. 4th Revised Edn. l992.

DETAILED SYLLABUS OF SEMESTER -III

Course Code	Course Name	L – T – P	**Credits**
AC 509	**ORGANOMETALLIC CHEMISTRY AND CATALYSIS**	3-0-2	**4**

Course Objectives:

To understand the basic of organometallics and their synthesis , bonding, properties and their applications

Course Contents

UNIT I: ORGANOMETALLICS

18-Electron rule, Oxidation state, co-ordination number and geometry. Effect of complexation with different metals (4d and 5d); Alkyls and hydrides: alkyls and aryls (metal alkyls stabilized carbanion, β-elimination, stable alkyls, agostic alkyls, reductive elimination, preparation of metal allyls). metal hydrides: characterization, synthesis, reactions, bridging hydrides.

UNIT II: SYNTHESIS, BONDING, PROPERTIES & APPLICATIONS OF ORGANOMETALLICS

Pi complexes, synthesis, bonding. Properties and application of alkenes and alkynes, allyls, diene, cyclopentane, dienyl, arenes. Distinctive organometallic Reactions - Addition and abstraction: Nucleophilic addition to CO, Nucleoplic addition to polynes and polyenyls, nucleophilic abstraction in hydrides, acyls, electrophilic addition and abstraction, single electron transfer and radical reactions, Oxidative – Addition reactions, Insertion reaction – at MC bond & M-H bond, Trans-metallation reaction and Cyclization reaction, Ring Expansion reaction, Condensation reaction, Sigma-pi rearrangement reaction, Ligand & Metal exchange reactions.. Fluxionality and dynamic equilibria,

UNIT III: TRANSITION METALS/ORGANOMETALLIC REAGENTS IN ORGANIC SYNTHESIS

Alkene isomerisation, hydrogenation, hydroformylation, hydrocyanation, hydroboration, coupling reaction. Carbon-carbon bond formation through coupling reactions – Heck, Suzuki, Stille, Sonogoshira, Negishi, Kumada, Hiyama, Tsuji-Trost, olefin metathesis and McMurry.

UNIT-IV: IMPORTANT ORGANOMETALLIC REACTIONS

Homogeneous catalysis –Catalytic applications of organometallic complexes - Alkene hydrogenation, Synthesis gas (H2/CO), Hydroformylation, Mosanto-acetic acid process, Wacker- Schmidt process and Ziegler-Natta catalysis. Bioorganometallic chemistry and surface organometallic chemistry.

Course Outcomes

After completing this course, the students will be able to:
CO1: To understand fundamentals of Organometallic chemistry
CO2: To familiarize with the synthesis, property studies and application of Organometallic chemistry
CO3: Applications of Organometallic reagents in Organic Synthesis

Text Books

1. Organometallics: A concise Introduction, Ch.Elshebroicn and A Salzer, VCH, 2006.

2. Organ transition Metal Chemistry: Applications to Organic Synthesis, S.G. Davies, Pergamon 1982.

Reference Books

Basic Organometallic Chemistry, Anil Elias

Course Code	Course Name	L – T – P	**Credits**
AC 510	**INDUSTRIAL CHEMISTRY**	3-0-2	**4**

Course Objectives: To understand the scalability of laboratory reactions in Industry with proper operations and safety.

Course Contents

UNIT I: CHEMICAL INDUSTRY

Introduction, Chemical production, Raw materials and their sources, Parameters of Chemical Industry, Plant location, Safety, Construction of plant, Management for productivity and creativity, Training for plant procedure and labour, Chemical process technology, Important chemical processes, Classification of chemical reactions, Batch and continuous operations, Industrial chemical reactions, Conversion, Selectivity and Yield, From Chemistry Laboratory to Industrial Scale

UNIT II: INDUSTRIAL PROCESSES AND THEIR SAFTEY:

Introduction, Unit operations- Conveying, Crystallization, Distillation, Drying, Evaporation, Filtration, Leaching, Liquid-liquid extraction, Membrane separation, Particle size reduction and enlargements, Solid -solid separation.

Introduction, Industrial unit processes- Definition and examples of Alkylation, Amination by amino lysis, Calcination, Carbonylation, Double decomposition, Esterification, Halogenation, Hydro formulation, Hydrolysis, Nitration, Oxidation, Polymerisation, Sulphonation.

Safety in Industry

UNIT III: AMINATION BY REDUCTION:

Introduction and definition, Methods of reduction, Metal and acid Reductions, Metal and alkali reductions, Amination by amino-lysis, aminating agents, physical and chemical factors affecting amino lysis, manufacture of aniline by reduction of nitrobenzene, p-phenylenediamine, aniline by continuous ammonolysis.

UNIT: IV IMPORTANT INDUSTRIAL REACTIONS

a) **INTRODUCTION AND TYPES** of Alkylation, alkylating agents, factors controlling alkylation, equipment for alkylation, alkylation methods for i) Alkyl-aryl sulphonates, ii) Ethylbenzene, iii) Dimethylaniline.

b) **HYDROLYSIS:** Definition and scope, hydrolyzing agents, materials susceptible to hydrolysis, kinetics, thermodynamics and mechanisms of hydrolysis, Equipment for hydrolysis, Technical operations involving hydrolysis.

c) **OXIDATION:** Liquid and vapour phase oxidations, apparatus for Oxidation, technical oxidation of acetaldehyde, iso-propyl alcohol, naphthalene, and naphthalene sulphonic acid.

   Esterification: Esterification of organic acids and derivatives, esters by addition, to unsaturated systems, interesterification of lard, technical preparation of ethyl acetate, cellulose acetate, nitroglycerol, polyethyl ether.

d) **HYDROGENATION:** Catalytic hydrogenation, Apparatus, Industrial processes, Hydrogenation of fatty oils, Synthesis of methanol.

   Nitration: Introduction, Nitrating reagents, Aromatic nitration, Nitration of paraffinic hydrocarbons, nitrate esters, N-nitro-compounds, process equipment for technical nitration, Mixed acid nitration, Typical Industrial nitration processes.

Course Outcomes

After completing this course, the students will be able to:
CO1: To understand the scalability of laboratory reactions in Industry
CO2: To understand operations and safety in Industrial reactions
CO3: Indepth study of Amination/Alkylation reactions

Text Books

1. Unit Processes in Organic Synthesis- P. H. Groggins, Tata McGraw-Hill, 5th

Edition, New Delhi, 2010.

2. Dryden's Outline of Chemical Technology, M. Gopal Rao, Marshall Sittig East-West Press Pvt. Ltd., 3rd Edition, 2014.
3. Chemical Process Industries- B. Shreve., Tata McGraw Hill, New Delhi, 2012.
4. Comprehensive Industrial Chemistry, P. G. More, Pragati Edition, Meerut, 2010.
5.

Reference Books

1. Encyclopaedia of Chemical Technology, Kirk and Othmer, John Wiley & Sons, 2000

SYLLLABUS OF ELECTIVE COURSES

Course Code	Course Name	L – T – P	**Credits**
AC 511	MOLECULAR SPECTROSCOPY-I	4-0-0	**4**

Course Objectives: to understand fundamental principles of Spectroscopy and theories involved

Course Contents

Basic elements of spectroscopy, Interaction of Radiation with matter, Time dependent perturbation. Einstein coefficients. Integrated absorption coefficients. Transition dipole moments and general selection rules based on symmetry ideas.

UNIT I: INTRODUCTION TO MOLECULAR SPECTROSCOPY

Rotational spectroscopy of diatomic molecules. Rigid rotor approximation. Determination of bond lengths and/ or atomic masses from microwave spectral data. Effect of isotopic substitution. Non-rigid rotator. Classification of polyatomic molecules. Energy levels and spectra of symmetric top molecules and asymmetric top molecules. First order Stark effect.

UNIT II: ATOMIC SPECTRA

Characterization of atomic states. Microstate and spin factoring methods. Hund's rules. Derivation of spin and orbital selection rules (based on recursion relations of Legand re polynomials). Spectra of complex atoms. Zeeman and Stark effects. Construction of hybrid orbitals using symmetry aspects. Atomic Spectroscopy: The energies of atomic orbitals; Hydrogen atom spectrum; Orbital and spin angular momenta, total angular momentum; the fine structure of hydrogen atom spectrum; The spectra of complex atoms: Singlet and triplet states; Russell-Saunders coupling; Term Symbols and selection rules. Franck-Condon principle, electronic and Raman spectroscopy of diatomic and polyatomic molecules.

UNIT IV: VIBRATIONAL SPECTROSCOPY

Homonuclear and heteronuclear diatomic molecules. Extension to polyatomic linear molecules. Derivation of selection rules for diatomic molecules based on Harmonic oscillator approximation. Force constants and amplitudes. A harmonic oscillator. Overtones and combination bands. Introduction to normal coordinate analysis.

Dissociation energies from vibrational spectral data. Vibration-rotation spectra, P, Q and R branches. Breakdown of the Born-Oppenheimer approximation. Nuclear spin effect.

Symmetry of normal coordinates. Use of Group Theory in assignment of spectra and selection rules for simple molecules.

Course Outcomes

After completing this course, the students will be able to:
CO1: To study understand the principles of atomic and molecular spectroscopy
CO2: To understand theory of vibrational spectroscopy

Text Books

BOOKS (MOLECULAR SPECTROSCOPY)

1. Introduction to Spectroscopy, Donald Pavia,
2. Spectrometric Identification of Organic Compounds, R. M. Silverstein, G. C. Bassler and T. C. Morrill, John Wiley & Sons, New York, 5th Ed.1991.
3. Electron Paramagnetic Resonance, Elementary Theory and Practical Applications, Weil, John A, J. R. Bolton, and Wertz, J. E, Wiley-Inter science, New York, (1994).
4. Structural Methods in Inorganic Chemistry, E.A.V. Ebsworth, D.W.H. Rankin, & S. Cradock, 2nd Ed.1991, CRC Press, Boca Raton, Florida,
5. Principles of Fluorescence Spectroscopy, Lackowicz, Plenum Press, (New York,1983)

Reference Books

D. W. Williams and Flemming, Spectroscopic methods of organic compound

Course Code	Course Name	L – T – P	**Credits**
AC 512	**MOLECULAR SPECTROSCOPY II**	3-0-2	**4**

Course Objectives:To understand and apply various spectroscopic techniques for characterization.

UNIT I: RAMAN SPECTROSCOPY

Stokes and anti-Stokes lines. Polarizability of molecules. Rotational and Vibrational Raman spectroscopy. Selection rules. Polarization of Raman lines.

UNIT II: ELECTRONIC SPECTROSCOPY

Diatomic molecules. Selection rules. Breakdown of selection rules. Franck-Condon factors. Dissociation energies. Photoelectron spectroscopy of diatomic (N2) and simple polyatomic molecules (H2O, formaldehyde). Adiabatic and vertical ionization energies. Koopmans' theorem. Qualitative ideas of solvent effects- viscosity, polarity, hydrogen bonding.

UNIT III: NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY (NMR)

General introduction and definition; chemical shift; spin–spin interaction; shielding mechanism of measurement; chemical shift values and correlation for protons bonded to carbons [aliphatic; olefinic; aldehydic and aromatic] and other nuclei [alcohols; phenols; enols; acids; amines; amides and mercaptans]; chemical exchange; effect of deuteration; complex spin-spin interaction between two; three; four; and five nuclei [first order spectra]; virtual coupling. Stereochemistry; hindered rotation; Karplus curve variation of coupling constant with dihedral angle. Application of ^{1}H and ^{13}C NMR spectroscopy including COSY, NOESY, NOE techniques in the structural determination of complex organic systems. Application in conformational analysis. Multinuclear NMR of various inorganic and organometallic compounds. Data Interpretation, case studies.

UNIT IV: ELECTRON SPIN RESONANCE

Electron spin and Magnetic moment, Resonance condition in ESR and significance of 'g' value. ESR spectra of organic free radicals, Mc Connel relation, Electron Exchange reactions, applications of ESR.

UNIT V: PRINCIPLES OF MOSSBAUER SPECTROSCOPY

Basic principles, a chirality of nucleus, Isomer shifts. Quadrupole and Nuclear Zeeman splittings. Applications in structure determination.

UNIT VI: ELECTRIC AND MAGNETIC PROPERTIED OF MOLECULES

Polarizability, polarization of a molecule in an electric field (electronic, atomic and orientation polarization), Clausius-Mossotti equation, variation of molar polarization with temperature: Debye equation, bond moments, dipole moments and molecular structure. Magnetic susceptibility, molecular interpretations of diamagnetism and paramagnetism, Ferro, ferri and antiferromagnetic behavior, Curie and Neel temperatures, Measurements of magnetic susceptibility by Faraday and Gouy Technique.

Course Outcomes

After completing this course, the students will be able to: **CO1:** To understand the principles of RAMAN spectroscopy **CO2:** To understand the principles of electronic spectroscopy **CO3:** To understand the principles of NMR spectroscopy **CO4:** To understand the principles of Mossbauer spectroscopy
Text Books
Reference Books

Course Code	Course Name	L – T – P	**Credits**
AC 513	**DEFENCE CHEMISTRY**	3-0-2	**4**
Course Objectives: To familiarize students about the utility of chemistry in defence			
UNIT I **Explosives:** Introduction, Classification, Nature of Explosives,Burning, Deflagration & Detonation, Initiation theories of explosives,Thermochemistry of explosives, various performance parameters of explosives, **Propellants:**Introduction, Rocket & Gun Propellants, **Pyrotechnics:** Definition, classification, Ingredient, Various compositions **UNIT II** Polymers and Nanocomposite for defence applications: Metal replacement polymers., High Performance Engineering Polymers, Lightweight polymers, Chemical Resistant polymers. **UNIT III** High Strength Materials, alloys for defence applications **UNIT IV**			

Nuclear Science: Structure of nucleus, Mass defect, Binding energy, Nuclear reactions, fission & Fusion nuclear reactions,Controlled & uncontrolled release of nuclear energy, Concepts of critical mass & critical volume

Chemical & Biological Weapons: Different chemical and Biological warfare agents & their effects; Protection against biological, chemical warfare agents

Text/References:

1) Principles/Effects & Sensitivity, 1994, C.S.Grace, Brasey series
2) Chemical warfare agents, 1992, S.M.Somai
3) Biological weapons, 1999, Joshua Lederberg

Course Outcomes

After completing this course, the students will be able to:
CO1: Study of chemistry of High Energy Materials
CO2: To understand the applications of polymers and nanocomposites in defence
CO3: To familiarize with High strength materials
CO4: To understand NBC and their remediation

Text Books

1. J P Agrawal: High Energy Materials, Wiley VCH, 2012
2. N. Ramdani: Polymer Nanocomposites for advanced Aerospace and Military Applications, IGI Global, 2019

Reference Books

1. NBC: Nuclear, Biological, and Chemical Warfare on the Modern Battlefield John Norris, Will Fowler, 1997.

Course Code	Course Name	L – T – P	**Credits**
AC-610	**RECENT ADVANCES IN CHEMISTRY**	3-0-2	**4**

Course Objectives:

UNIT-1. INTRODUCTION

Background and eminent discoveries in Chemical Technology Frontiers in Electrochemistry: Equilibrium properties of electrolytes, electrode potential, electro analytical techniques.

UNIT-2. GREEN CHEMISTRY

Principals of green chemistry, sustainability, selected examples of green synthesis.

Unit-3. Biochemistry & Biotechnology: Cell Biology and Physiology, Bioenergetics, Industrial Biotechnology.

Unit-4. Chemistry of smart materials: Smart materials, their properties, distribution by type chemistry of macromolecules, phase change materials

Course Outcomes

After completing this course, the students will be able to:
CO1: To familiarize students in important discoveries of chemical technologies
CO2: To understand electrochemical techniques
CO3: To understand biochemistry and biotechnology
CO4: To understand the chemistry of smart materials
CO5:

Text Books

1. Electrochemistry for Chemists, Sawyer, Sobkowiak, & Roberts, John Wiley, 1995.
2. Concepts in Transition Metal Chemistry, Crabb, Eleanor, Moore, Elaine, Smart, Lesley E.RSC Publishing, 2010
3. Highlights in Bioorganic Chemistry, Carsten Schmuck, HelmaWennemers, Wiley-VCH, 2004.
4.

Reference Books

1. Essentials of Pharmaceutical Chemistry, D. Cairns 5. Intelligent Materials, M. Shahinpoor, H.-J. Schneider, RSC, 2008

Course Code	Course Name	L – T – P	**Credits**
AC 611	**<u>QUANTUM CHEMISTRY</u>**	3-0-2	**4**
Course Objectives:			

<u>UNIT I: QUANTUM CHEMISTRY-I</u>

Basic postulates of Quantum mechanics (a brief review). Operators in Quantum mechanics: Linear and Hermitian operators, Commutation of operators. Differential equations, partial differential equations, series solutions and special functions, linear vector spaces, transformation of coordinate matrix, representation of operators, eigenvalue problem, orthonormal sets, Fourier and Laplace transforms. Some exactly soluble problems. Simple harmonic oscillator problem. Calculation of various average values using ladder operators and recursion relations of Hermite polynomials. Angular momentum operators. Eigenvalues and eigenfunctions. First order time-independent perturbation theory for non-degenerate states. Variation theorem, variational methods and their applications. Ground and excited state of helium atom.

UNIT II: QUANTUM CHEMISTRY-II

Schrodinger equation for hydrogen atom and its solution, the origin of electronic quantum members and physical significance - radial probability density significance of magnetic quantum number with respect to angular momentum. Hydrogen molecule ion and hydrogen molecule Paulis exclusion principle. Term symbols for electronic state in atoms– LS and JJ coupling. Born Oppenheimer approximation, Variational treatment of hydrogen molecule ion. Mulliken designation of molecular orbitals, wave functions for many electron atoms– Hartres–Fock SCF method, Slater Orbitals.

Unit III: Born interpretation. Dirac braket notation. Particle in a box: infinite and finite square wells; concept of tunnelling; particle in 1D, 2D and 3D-box; applications. Harmonic oscillator: harmonic and an harmonic potentials; hermite polynomials. Rotational motion: Angular momentum operators, Rigid rotor. Hydrogen and hydrogen-like atoms: atomic orbitals; radial distribution function. Multi-electron atoms: orbital approximation; electron spin; Pauli exclusion principle; slater determinants. Approximation Methods: Variation method and secular determinants; first order perturbation techniques. Atomic units. Molecular structure and Chemical bonding: Born-Oppenheimer approximation; Valence bond theory and linear combination of atomic orbitals –molecular orbital (LCAO-MO) theory. Hybrid orbitals. Applications of LCAO-MO theory to H_2+, H_2; molecular orbital theory (MOT) of homo- and heteronuclear diatomic molecules. Hückel approximation and its application to annular π– electron systems.

Course Outcomes

After completing this course, the students will be able to:
CO1: To understand the basics of Quantum Chemistry and various laws in this regard
CO2: Familiarize with important concepts to hypothise quantum mechanics
CO3: To understand important postulates of quantum chemistry

Text Books

1. I. N. Levine, 'Quantum Chemistry', 4th Edn., Prentice Hall India, 2001.

2. A. K. Chandra, Introductory Quantum Chemistry, Tata McGraw Hill 1994.

3. M.S. Gopinathan and V. Ramakrishnan, Group Theory in Chemistry, Vishal Publishers,1988.

4. Methods of Molecular Quantum Mechanics by P.W. Atkins.

5. Cotton, F.A. Chemical Applications of Group Theory, 3rd Edn., John Wiley and Sons, 2003.

6. Physical Chemistry: A Molecular Approach by D.A. Mc Quarrie and J.D. Simon

7. D.A. McQuarrie. Quantum Chemistry, Viva Books Pvt Ltd (2003)

8. Jack Simons, Introduction to Theoretical Chemistry, Cambridge University Press, 2003.

Reference Books

P.W. Atkins. Molecular Quantum Mechanics, Oxford University Press (1986)