SMIT SIKKIM MANIPAL UNIVERSITY

SIKKIM MANIPAL INSTITUTE OF TECHNOLOGY

M.Sc. Chemistry Syllabus Revision-2022
B. Tech Engineering Chemistry Syllabus Revision-2022
B. Tech Environmental Science Syllabus Revision-2022

DEPARTMENT OF CHEMISTRY
SIKKIM MANIPAL INSTITUTE OF TECHNOLOGY
MAJHITAR, RANGPO, EAST - SIKKIM, INDIA

SIKKIM MANIPAL UNIVERSITY

VISION:

- Global Leadership in Human Development, Excellence in Education and Healthcare.

MISSION:

- Develop professionals of excellent technical calibre in the field of Health Sciences, Engineering, Management and Social Sciences with a humane approach capable of shouldering the responsibility of building the nation and be globally competent.

OBJECTIVE:

- To support, promote and undertake the advancement of academics.
- To promote use of ICT and modern education technologies.
- To encourage research, creation and dissemination of knowledge.
- To facilitate extension and community service.
- To empower people of Sikkim and contribute to human development in Northeast.
- To create environmental and social responsibilities among students and employees.
- To ensure steady growth of the University.

SIKKIM MANIPAL INSTITUTE OF TECHNOLOGY

VISION:

- To achieve eminence in the field of quality technological education and research.

MISSION:

- To develop SMIT into an Institution of Excellence capable of producing competent techno-managers who can contribute effectively to the advancement of the society.

OBJECTIVE:

- To provide wholesome education to meet the intellectual aspirations of the students.
- To equip students with techno-managerial skills to enable them to take their assigned role in the industry.
- To inculcate essential ethics and values to meet the spiritual needs to the students.
- To provide a sound institutional environment nurturing emotional strength, healthy mind, body and resilience amongst the students.

DEPARTMENT OF CHEMISTRY

VISION:

- To emerge as a centre of excellence in teaching and research.

MISSION:

- To equip the students with latest knowledge in science and technology such as to contribute as valuable members of the society.

OBJECTIVE:

- To provide quality teaching and research.
- Inculcate societal responsibility in the students.
- To provide sufficient training in terms of latest developments in the field of chemistry.

PO's

1. Develop and refine fundamental knowledge of Chemistry.
2. Cultivate in –depth knowledge in Organic chemistry, Inorganic chemistry, Physical chemistry, Analytical chemistry and Spectroscopy.
3. To improve analytical and logical capability so as to import the ability to solve new and complex problems.
4. Developing the team work philosophy.
5. Imbibing research acumen and innovative thinking so as to become a good researcher.
6. Motivating and developing the knack for clearing competitive exams.
7. Developing presentation skill and improving / fine tuning personal interaction.
8. To use the knowledge for the betterment of the society.
9. Aquire hands on experience in experimental chemistry.

PSO

1. To develop up-to-date knowledge in different fields of chemistry.
2. Ability to carry out challenging research work in the frontier areas.
3. Ability to use spectroscopic techniques for analysis.
4. Good communication and presentation skills.
5. To evolve into a good person, commitment towards society.

PEO

1. To motivate and prepare post graduate students through effective coaching for higher education and research.
2. To impart education and training to the students for better employment.

ANNEXURE I

Department of Chemistry

Summary of Syllabus Revision-2022

M.Sc. Chemistry Syllabus Revision-2022

Old Sub Code	Sub Code	Sub Name	% of Modification	Effective from
CH2101	CH20101A	Principles of Inorganic Chemistry	Divided in 5 Modules	August 2022
CH2102	CH20102A	Principles of Organic Chemistry	Divided in 5 Modules	August 2022
CH2103	CH20103A	Chemical Thermodynamics	Divided in 5 Modules	August 2022
CH2104	CH20104A	Analytical Chemistry	Divided in 5 Modules	August 2022
CH2161	CH20401A	Analytical Chemistry lab	No Modification	August 2022
CH2162	CH20402A	Physical Chemistry lab	No Modification	August 2022
CH2201	CH20105A	Modern Spectroscopic Technique	Divided in 5 Modules	January 2023
CH2202	CH20106A	Organic Reactions and Mechanisms	Divided in 5 Modules	January 2023
CH2203	CH20107A	Computer Fundamentals & Programming	Divided in 5 Modules	January 2023
CH2204	CH20108A	Quantum Chemistry- I	Divided in 5 Modules	January 2023
CH2261	CH20403A	Computer Programming Lab	No Modification	January 2023
CH2262	CH20404A	Organic Chemistry Lab	No Modification	January 2023
CH2301	CH20109A	Advanced Coordination Chemistry & Inorganic Reaction Mechanism	Divided in 5 Modules	August 2022
CH2302	CH20110A	Concepts in Organic Synthesis	Divided in 5 Modules	August 2022
CH2303	CH20111A	Chemical Dynamics and Electrochemistry	Divided in 5 Modules	August 2022
CH2304	CH20112A	Biochemistry	Divided in 5 Modules	August 2022
CH2331	CH20301A	Photoinorganic Chemistry	Divided in 5 Modules	August 2022
CH2332	CH20302A	Synthetic Organic Chemistry	Divided in 5 Modules	August 2022
CH2333	CH20303A	Advanced Physical Chemistry	Divided in 5 Modules	August 2022
CH2361	CH20405A	Inorganic Chemistry Lab	No Modification	August 2022
CH2401	CH20113A	Bio-inorganic Chemistry	Divided in 5 Modules	January 2023

CH2402	CH20114A	Solid State Chemistry and Interface Science	Divided in 5 Modules	January 2023
CH2403	CH20115A	Group Theory–A Chemist Approach	Divided in 5 Modules	January 2023
CH2404	CH20116A	Quantum Chemistry- II	Divided in 5 Modules	January 2023
CH2475	CH20601A	Research Project work		January 2023
CH2431	CH20304A	Chemistry of Nanomaterials	Divided in 5 Modules	January 2023
CH2432	CH20305A	Supramolecular Chemistry	Divided in 5 Modules	January 2023
CH2433	CH20306A	Medicinal Chemistry	Divided in 5 Modules	January 2023

B. Tech: Engineering Chemistry Syllabus Revision-2022

Old Sub Code	Sub Code	Sub Name	% of Modification	Effective from
CH1108	CH10101A	Engineering Chemistry	15% Divided in 5 Modules	August 2022
CH1163	CH10401A	Engineering Chemistry Lab	No Modification	August 2022

B. Tech: Environmental Science Syllabus Revision-2022

Old Sub Code	Sub Code	Sub Name	% of Modification	Effective from
CH1191	CH10102A	Environmental Science	Divided in 5 Modules	August 2022

DEPARTMENT OF CHEMISTRY			
M.Sc. (CHEMISTRY) 1st Semester			
Sl. No.	**Sub Code**	**Sub Name**	**Credit**
1.	CH20101A	Principles of Inorganic Chemistry	4
2.	CH20102A	Principles of Organic Chemistry	4
3.	CH20103A	Chemical Thermodynamics	4
4.	CH20104A	Analytical Chemistry	4
5.	CH20401A	Analytical Chemistry Lab	3
6.	CH20402A	Physical Chemistry Lab	3
7.	CH20601A	Project Based Seminar	1
		Total Credit for this semester	**23**
M.Sc. (CHEMISTRY) 2nd Semester			
1.	CH20105A	Modern Spectroscopic Technique	4
2.	CH20106A	Organic Reactions and Mechanisms	4
3.	CH20107A	Computer Fundamentals & Programming	4
4.	CH20108A	Quantum Chemistry- I	3
5.	CH20403A	Computer Programming Lab	3
6.	CH20404A	Organic Chemistry Lab	3
7.	CH20602A	Project Based Seminar	1
		Total Credit for this semester	**22**
M.Sc. (CHEMISTRY) 3rd Semester			
1.	CH20109A	Advanced Coordination Chemistry & Inorganic Reaction Mechanism	4
2.	CH20110A	Concepts in Organic Synthesis	4
3.	CH20111A	Chemical Dynamics and Electrochemistry	4
4.	CH20112A	Biochemistry	4
5.	EL-I	Elective I (special paper)	4
6.	CH20405A	Inorganic Chemistry Lab	3
7.	CH20603A	Project Based Learning	1
		Total Credit for this semester	**24**
M.Sc. (CHEMISTRY) 4th Semester			
1.	CH20113A	Bio-inorganic Chemistry	4
2.	CH20114A	Solid State Chemistry and Interface Science	4
3.	CH20115A	Group Theory – A Chemist Approach	4
4.	CH20116A	Quantum Chemistry- II	4
5.	EL-II	Elective II (Special Paper)	4
6.	CH20604A	Research Project Work	6
		Total Credit for this semester	**26**
ELECTIVE I			
1.	CH20301A	Photoinorganic Chemistry	4

2.	CH20302A	Synthetic Organic Chemistry	4
3.	CH20303A	Advanced Physical Chemistry	4
ELECTIVE II			
1.	CH20304A	Chemistry of Nanomaterials	4
2.	CH20305A	Supramolecular Chemistry	4
3.	CH20306A	Medicinal Chemistry	4
		M.Sc. Chemistry Total Credit	**95**

B. TECH 1st Year			
Sl. No.	**Sub Code**	**Sub Name**	**Credit**
1.	CH10101A	Engineering Chemistry	4
2.	CH10401A	Engineering Chemistry Lab	1
3.	CH10102A	Environmental Science	0

Syllabus Revision
2022

- M.Sc. Chemistry
- B. Tech Engineering Chemistry
- B. Tech Environmental Science

Department of Chemistry
Sikkim Manipal Institute of Technology

ANNEXURE II

M.Sc. Syllabus Revision – 2022

Principles of Inorganic Chemistry
Subject Code: CH20101A (with effect from August 2022)

Credit 4 **Contact hours:** 4 hrs/week

Objective: The course aims to strengthen the fundamentals of inorganic chemistry covering main group elements and inner transition elements.

Course Outcome:
CO1: In-Depth knowledge of periodic properties of elements, structure and bonding in molecules. Ability to assign structure and deduce properties of a given molecules.
CO2: Ability to explain acid base concept, magnetic properties of molecules, and their application in deducing properties of a molecule.
CO3: In-Depth knowledge of synthesis, properties bonding of p- block elements and their compounds and applications.
CO4: In-Depth knowledge of synthesis, properties bonding of Boranes, Carboranes, Metallocarboranes, Borazines, Phosphazenes, Sulfur-Nitrogen compounds, silicates, silicones. Iso- and Hetero-poly anions. Understand the concept of allotropy and its significance.
CO5: In-Depth knowledge of Metal-Metal bonds, industrial importance of the compounds of main group elements. Brief review of inorganic chains, rings and cages, organometallic compounds of non-transition elements.

Module - I

Periodicity: Ionization Energy, Electron Affinity, Electronegativity.
Structure and bonding in homo- and heteronuclear molecules: VSEPR Theory, VBT, Bent's rule, Fajan's rule, MOT, physical properties of molecules (bond energies, force constants, bond lengths bond polarities and electronegativity). **(8 hrs)**

Module - II

Concepts of acids and bases, Lewis acids and bases, Hard-Soft acids and bases, HSAB principle, Chemistry in Non-aqueous solvents.
Magnetic properties, paramagnetism, ferro and antiferro magnetism, diamagnetism, determination of magnetic susceptibility.
Inner transition elements: spectral and magnetic properties, redox chemistry, analytical applications. **(8 hrs)**

Module - III

Main group elements and their compounds: Synthesis, Properties, Structure and Bonding of: Nitrogen, Phosphorous, Oxygen, Sulfur, Selenium, Pseudohalogen, Interhalogen and Xenon Compounds. **(8 hrs)**

Module - IV

Boranes, Carboranes, Metallocarboranes, Borazines, Phosphazenes, Sulfur-Nitrogen compounds, silicates, silicones. Iso- and Hetero-poly anions, Allotropy. **(8 hrs)**

Module -V

General Periodic trends among Metals, compounds containing Metal-Metal bonds, industrial importance of the compounds of main group elements. Brief review of inorganic chains, rings and cages, organometallic compounds of non-transition elements. **(8 hrs)**

Texts Books / Reference Books:

1. Inorganic Chemistry, Principles of Structure and Reactivity - James E. Huheey, Ellen A. Keiter, Richard L. Keiter
2. Advanced Inorganic chemistry – F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochman
3. Inorganic Chemistry - Shrivers and Atkins
4. Inorganic Chemistry – G. L. Miessler, P. J. Fischer & D. A. Tarr

Principles of Organic Chemistry
Subject Code: CH20102A (with effect from August 2022)

Credit 4 **Contact hours:** 4 hrs/week

Objective: This course gives the idea of MO's theory, acid-base concept, stereochemistry, Organic reaction intermediate and substitution reactions (Aliphatic and Aromatic).

Course Outcome:
CO1: Ability to use MOT for predicting reaction mechanism
CO2: Able to solve problems related with stereochemistry
CO3: Able to use acidic and basic conditions for carrying out suitable reactions
CO4: Understanding of role of reaction intermediate in organic synthesis and nucleophilic substitution reaction.

Module - I

Principle of MO's theory and its application to reactivity

Introduction, Molecular orbital - homonuclear, heteronuclear (both sigma and pi-bonded molecule), delocalization, tautomerism, aromaticity, anti-aromaticity etc. Huckel molecular orbital theory. **(3 hrs)**

Stereochemistry - I

Isomers – Classes of isomers, Isomerism – optical and geometrical Isomerism, Nomenclature of enantiomers – R.S. & E.Z. system**.** **(5 hrs)**

Module -II

Stereochemistry - II

Elements of symmetry, Concept of chirality, Centre of chirality - molecules with C, N, S based chiral centers, molecules with more than one chiral center, Projection formulae (i) Fischer (ii) Sawhorse (iii) Newman (iv) Flying wedge and their interconversions; threo and erythro isomers, methods of resolution, optical activity in absence of chiral carbon, atropisomerism.

Conformational analysis of cycloalkanes: Meaning of conformation, Effect of conformation on the stability and reactivity, Stereochemistry of six membered rings, Mono substituted and disubstituted cyclohaxane, Decalines, Gauch butane interactions in substituted cyclohexanes and decalines. **(8 hrs)**

Module -III

Concept of Acids and Bases

Introduction about acids and bases (lewis theory), Concept of pK_a and pK_b, Origin of the acidity and basicity with various factors, acid and bases catalysis, Application of pK_a in nucleophilic substitution reaction, Application of HSAB principle in organic reactions. **(3 hrs)**

Reactive intermediates - I

Carbocation: Structure, and stability of carbocations, Classical and non-classical carbocation, C-C bond formation involving carbocations, Oxymercuration, halolactonisation. Acetal formation, Friedel-crafts reaction, Wagner-Meerwein rearrangement, Hydroperoxide rearrangement. **(5 hrs)**

Module -IV

Reactive intermediates - II

Carbanion: Structure and stability, Chemistry of enolates and enamines, Kinetic and thermodynamic enolates, alkylation and acylation of enolates, Nucleophilic additions to carbonyls, Introduction of Favorskii and Neber rearrangement.

Free radicals: Generation, structure, and stability of radical intermediates and their (a) addition to alkenes, alkynes (inter & intramolecular) for C-C bond formation (b) fragmentation and rearrangements.

Carbenes: Generation, structure and stability, Addition and insertion reactions. **(8 hrs)**

Module –V

Reactive intermediates - III

Nitrenes: Generation, structure and stability, Reactions of nitrene and related electron deficient nitrogen intermediates, Hoffmann, Schmidt, Beckmann rearrangement reactions. Curtius rearrangement –mechanism challenges. Effect of structure on reactivity, The Hammett equation and linear free energy relationship (sigma-rho), Taft equation. **(4 hrs)**

Aliphatic & Aromatic Neucleophilic Substitutions:

The S_N1, S_N2 mechanisms, factors affecting the mechanism, neighbouring group effect, S_Ni, $S_N!$ /, S_N2 /, Nucleophilic substitution at an allylic, vinyl carbon, Nucleophilic aromatic substitutions, Benzyne, S_NAr mechanism. **(4 hrs)**

Texts Books / Reference Books:

1. Organic Chemistry, vol. I & II (ELBS)- Finar, I.L
2. Advanced Organic Chemistry -J. March, Willey Interscience
3. Organic Chemistry - O.P. Agrawal
4. A Guidebook to Mechanism in Organic Chemistry by Peter Sykes
5. Stereochemistry – Eliel
6. Stereochemistry – D. Nashipuri
7. Organic Chemistry – J. Clayden, N Greeves, S. Warren & P. Wothers

Chemical Thermodynamics
Subject Code: CH20103A (with effect from August 2022)

Credit 4 **Contact hours:** 4 hrs/week

Objective: The study of entropy, free energy and work function relation with the change of various conditions and their mathematical application to understand third law, chemical potential, the phase equilibrium and statistical thermodynamics.

Course Outcome:

CO1: To impart fundamental concepts of solution thermodynamics involving ideal and non-ideal systems.

CO2: To use solution thermodynamic concepts and phase equilibria in two-component and multi-component systems.

Module I

Entropy, Gibbs & Helmholtz Free energy functions & their variation with various conditions, Maxwell thermodynamic relation. **(8hrs)**

Module II

Clapeyron Clausius equation with derivation & application to various phase equilibrium, & Colligative properties - elevation of boiling point and depression of freezing points, Van't Hoff law of mass action & reaction isotherm, isochore with different methods, Raoult's law and its application. **(6hrs)**

Module III

Limitation of Gibb's Helmholtz concepts, Nernst heat theorem, its proof and application, Third law of thermodynamics, its application and exception of third law. **(6hrs)**

Module IV

Partial molar properties & their determination, Chemical potential of gas for pure ideal & in mixture and its application. **(4hrs)**

Gibbs Duhem equation for open system, Thermodynamic criteria for equilibrium in open system, Concept of Fugacity & Activity, their significance, variation of Fugacity & Activity of a gas with pressure and temperature. **(6hrs)**

Module V

Phase rule and its thermodynamic derivation, Application of phase rule and treatment of Clapeyron Clausius equation in one component system. Phase diagram of -one component system **as** H_2O, Sulphur, carbon di oxide - two component systems, binary liquid systems. **(5hrs)**

Reduced Phase rule, Eutectic systems as lead silver system, potassium iodide-water system, Binary alloys system with congruent and incongruent melting points. **(5hrs)**

Texts Books / Reference Books:

1. Advance Physical Chemistry – D.N.Bajpai
2. Physical Chemistry – Silbey & Alberty
3. Physical Chemistry – Atkins
4. Physical Chemistry of Molecular Approach – Mc. Quarrie & Simon
5. Fundamentals of classical and Statistical Thermodynamics-B.N.Roy
6. Classical and Statistical Thermodynamics- A.H.Carter

Analytical Chemistry
Subject Code: CH20104A (with effect from August 2022)

Credit 4 **Contact hours:** 4 hrs/week

Objectives: The course aims to introduce students to the fundamental principles of Analytical Chemistry. The course introduces the concept of errors and correct techniques for sampling and then delves into the various aspects of analytical chemistry viz, chemometrics, separation techniques followed by analytical techniques including instrumental methods of analysis.

Course Outcome:
CO1: Understand the principles of Chemometrics.
CO2: Understand the underlying principles, techniques, data analysis of Seperation techniques and quantitative analysis.
CO3: Ability to apply chemical analysis techniques for determining composition of samples.
CO4: Interpret and optimize results.

Module –I

Introduction to Analytical chemistry, **Errors**, classification of errors, determining and improving of accuracy in analysis, mean, median, mode, standard deviation, coefficient of variation, Confidence interval, Comparison of results, student t-test, F test, Q test, rejection of results, Correlation and Regression. **(8hrs)**

Module –II

Separation Techniques: Principle of solvent extraction, classification and mechanism of extraction, extraction by chelation and solvation, extraction equilibria, technique of extraction. Nomenclature of extractants.
Ion exchange Separations: synthesis of ion exchange resin, mechanism of ion exchange and equilibria, Applications of ion exchange. **(8hrs)**

Module –III

Chromatography: introduction to chromatography, classification, development of chromatograph, dynamic of chromatography, Plate theory for chromatography, VanDeemeter Equation**.** Thin layer chromatography, Gas chromatography – Principles, instrumentation and application, High Performance Liquid chromatography- Principles, instrumentation and application. **(8hrs)**

Module –IV

Solubility, solubility product, fractional precipitation, quantitative effects of common ion. degree of dissociation of weak acids and bases.
Gravimetric analysis, precipitation methods, purity of precipitate (co precipitation), optimum condition for precipitation, precipitation from homogeneous solution, washing and ignition of the precipitate, role of organic precipitate, criteria for choice of organic reagent, important organic precipitants. Numerical problems based on gravimetric analysis of mixtures.
Thermal Methods of Analysis: Thermogravimetric Analysis, DTA, DSC Instrumentation, Principles and their applications. **(8hrs)**

Module –V

Titrimetric analysis: classification, theory of indicators of each class of titrations, Titration curves for each class of titrations, Selectivity and Masking. Role of instruments in titration**.** **(8hrs)**

Texts Books / Reference Books:

1. Analytical Chemistry – S.M. Khopkar
2. Vogel'sQuantitative Chemical Analusis – J Mendhan, RC Denncy, JD Barnes, MJK Thomas
3. Instrumental methods of analysis – Willard, Merit & Dean
4. Analytical Chemistry – Gray D. Christian

Analytical Chemistry Lab
Subject Code: CH20401A

Credit: 3 **Contact hours:** 6 hrs/week

Objectives: The course aims to enable the students to apply the principles of analytical chemistry to the analysis of unknown chemical samples. This course is meant to complement the theoretical course.

Course Outcome:
CO1: Independently perform separation of components.
CO2: Perform accurately volumetric and gravimetric analysis.
CO3: Ability to analyse results.

List of Experiment of Analytical Chemistry Laboratory

1) Volumetric Analysis
   i) Acid - Base – Neutralization
   ii) Redox Titration (Including Iodometric Titration)
   iii) Precipitation Titration
   iv) Complexometric Titration

2) Gravimetric Analysis: At least one experiment involving each of the following:
   i) High temperature ignition compounds
   ii) Use of organic precipitants
   iii) Precipitation from Homogenous solutions

3) Solvent Extraction Experiments (Separation Volumetric Analysis may be combined)

4) Flame Photometry
   i) Estimation of Na^+
   ii) Estimation of K^+
   iii) Estimation of Na^+ and K^+ in a mixture

5) Spectrophotometric Analysis: Iron and Copper

6) Demonstration of the following experiments:
   i) TGA & DSC
   ii) Cyclic Voltammetry
   iii) Florescence Spectroscopy

Texts Books / Reference Books:

1. Analytical Chemistry – S.M. Khopkar
2. Vogel'sQuantitative Chemical Analusis – J Mendhan, RC Denncy, JD Barnes, MJK Thomas
3. Instrumental methods of analysis – Willard, Merit & Dean
4. Analytical Chemistry – Gray D. Christian

Physical Chemistry Laboratory
Subject Code: CH20402A

Credit: 3 **Contact hours:** 6 hrs/week

Objectives: The course aims to enable the students to understand the practical aspects of Physical Chemistry.

Course Outcome:
CO1: Ability to apply basic techniques of solution preparation and determine the aggregation process through Viscometric and conductometric methods.
CO2: Understand the experimental procedure to determine the kinetic parameters of selected reactions.
CO3: Ability to apply the knowledge of conductometric and potentiometric titration for determination of solubility of sparingly soluble salts.
CO4: Ability to determine the composition and complex formation through spectroscopic analysis.

Students are required to perform 15 experiments.

Study of Physical Properties:
1. Viscometric determination of average molecular weight of a high polymer.
2. Determination solubility product of lead iodide
3. Determination of transport number of Copper ion in solution by Hittrof's methods
4. To determine the transport number using moving boundary methods.
5. To determine the magnetic susceptibility by Guoy Balance.
6. Determination of electrophoretic mobility of AgI colloid.
7. Determination of partial molal volume of methanol in dilute aqueous solution.
8. Determination of CMC of surfactant molecule.
9. Determination heat of solution from solubility.

Kinetics Study:
1. Determinations of rate constant of alkaline hydrolysis of ethyl acetate.
2. Specific rate constant of inversion of cane sugar
3. Determination of rate law and the effect of temperature for the oxidation of iodine on Hydrogen Peroxide
4. Iodination of Acetone- Zero order kinetic
5. Homogeneous Chemical Equilibrium in Solution.

Conductometric Titration:
1. Cell constant determination
2. Acid base titration (monobasic and dibasic acids)
3. Precipitation titration ($AgNO_3$ vs KCl)
4. Determination of the solubility and solubility product of a sparingly soluble salt, conductometrically.

Potentiometric Titration:
1. Determination of E^0 of quinhydrone electrode
2. Acid base titration (HCl vs NaOH; $(COOH)_2$ vs NaOH; CH_3COOH vs NaOH)
3. Precipitation titration ($AgNO_3$ vs KCl)
4. Oxidation-reduction titration ($K_2Cr_2O_7$ vs Fe^{2+} ion)
5. Determination of Pka of Benzoic acid.
6. Acid-Base titration using pH meter.

Spectrophotometric Analysis:
1. Verify Beer's law for solution of $KMnO_4$ and $K_2Cr_2O_7$ using a spectrophotometer in their solution of unknown concentration.
2. Determination of copper ion by spectrophotometric methods.
3. Study of the complex formation between Ni and 1, 10-phenanthroline.
4. Determination of indicator constant by spectrophotometric methods.
5. Determination of composition and stability constant of a complex formed between Fe_3^+ ion and salicylic acid by Job's method.

Texts Books / Reference Books:

1. Experimental Physical Chemistry – V.D.Athawale & Parul Mathur
2. Practicals in Physical Chemistry – A Modern Approach-P.S.Sindhu
3. Experimental Physical Chemistry – Shoemaker & Nibler
4. Experimental Physical Chemistry – Farrington Daniels
5. Findlay's Practical Physical Chemistry- B.P.Levitt

Modern Spectroscopic Techniques
Subject Code: CH20105A (with effect from January 2023)

Credit 4 **Contact hours:** 4 hrs/week

Objective: Introduction to various techniques of spectroscopy used in chemistry. Detailed interpretation of spectra to identify unknown compounds. Introduction to advanced techniques for interpretation of complex spectra.

Course Outcome:
CO1: Understanding fundamentals of spectroscopy and ability to solve numerical problems (Determination of spectroscopic quantities, molar absorption coefficient).
CO2: Understanding fundamentals of rotational spectroscopy, interpret spectra and solve numerical problems. (Determination of rotational constants Bond Length).
CO3: Understanding fundamentals of vibrational spectroscopy, interpret spectra and solve numerical problems. (Force constant/Bond Energy).
CO4: Understanding fundamentals of Electronic spectroscopy of atoms and molecules, interpret spectra and solve numerical problems.
CO5: Understanding fundamentals of NMR and EPR spectroscopy, interpret spectra and solve numerical problems.

Module I

Introduction to molecular spectroscopy: Characterization of electromagnetic radiation, quantization of energy, S/N ratio, width and spectral intensity of spectral transition, F.T. Spectroscopy, stimulated emission. Types of molecular spectroscopy different types of molecular energies, Boltzmann distribution. **(4 hrs)**

Module II

Microwave spectroscopy – Rotational energy level, selection rule, Simple Harmonic Oscillator, Anharmonic Oscillator, Bond-distance of a diatomic molecule, relative population and intensity of the absorption peaks, Polyatomic molecules, limitations of microwave spectroscopy. **(6 hrs)**
Infrared spectroscopy - Introduction, the range of infrared spectroscopy, theory of I.R., SHO, vibrating diatomic molecule as anharmonic oscillator, diatomic molecule as a harmonic oscillator and a rigid rotator, interaction of rotations and vibrations, polyatomic molecules, limitations of I. R. spectroscopy. **(6 hrs)**

Module III

Electronic Spectroscopy of Atoms – Electronic wave functions, energies of atomic orbitals, electronic angular momentum, hydrogen atom spectrum, spectrum of many electron atoms, term symbols, microstate table, photoelectron spectroscopy, Zeeman effect. **(4 hrs)**

Module IV

Electronic Spectroscopy of Molecules – Born-Oppenheimer Approximation, vibrational-electronic spectra, Franck Condon Principle, dissociation energy and products, fine structure, Fortrat diagram, change of shape on excitation, chemical analysis by electronic spectroscopy. **(6 hrs)**

Module V

Spin Resonance Spectroscopy – NMR; NMR absorption by nuclei. Theory of NMR spectra, Spin-Spin and Spin-Lattice Relaxation, Multiple Pulse FT, chemical shift, shielding effects, deshielding effects, coupling constant, exchange phenomena, simplification of complex spectra, 13C NMR, Spectroscopy - double resonance. Application- structure determination, Keto-enol Tautomerism, limitations of NMR spectroscopy. **(10 hrs)**
Electron paramagnetic resonance **–** A brief introduction to epr. **(2 hrs)**
Identification of unknown molecule using combination of various type of spectra. **(2 hrs)**

Texts Books / Reference Books:

1. Fundamentals of Molecular Spectroscopy – C.N. Banwell and E.N. McCash
2. Spectroscopic Methods in Organic Chemistry – H. D. Williams and I. Flemming
3. Introduction to Spectroscopy – D. L. Pavia, G. M. Lampman and G. S. Kriz
4. Organic Spectroscopy – William Kemp

Organic Reactions And Mechanisms
Subject Code: CH20106A (with effect from January 2023)

Credit 4 **Contact hours:** 4 hrs/week

Objective: This course will give the idea about organic reaction mechanism, elimination and addition reaction, aromaticity. This will also highlight molecular rearrangement reactions.

Course Outcome:
CO1: Build up a strong foundation on various aspects of a reaction mechanism to establish it.
CO2: A clear conceptual understanding on various phenomena of organic compounds (especially unsaturated system)/intermediates through MOT.
CO3: A detail understanding about rearrangement reactions based on substrate nature & reaction condition and their reaction path.
CO4: A comprehensive knowledge on elimination reaction bases on substrate nature, used reagents and reaction conditions in organic synthesis.
CO5: Develop a power to reason, creative thought on elimination reaction based on substrate nature and reaction condition.

Module I

Mechanism and its investigation
a) Introduction, Energy profile diagram, Thermodynamics and kinetics requirement for reactions, Thermodynamic vs kinetic control, Hammond's postulate. Methods of determining mechanism - characterization of intermediate, nature of products, solvent effect, isotope effect, kinetic evidence, stereochemical evidences, microscopic reversibility**,** conclusion. **(6 hrs)**

Module II

Aromaticity: Annulene (Benzenoid and Non-benzenoid), Aromaticity in charged ring, Homoaromaticity, Fused ring system, Heterocyclic ring. Aromatic Electrophilic Substitution: Role of sigma- and pi- complex in aromatic electrophilic substitution, Electrophilic substitution reaction of Benzene- Nitration, Halogenation, Friedel-Craft reaction, Sulphonation, Mercuration. Effect of substituent, the ortho-para ratio, Substitution in disubstituted benzenes- competition between substituents. **(7 hrs)**

Module III

Molecular Rearrangement: 1,2-Rearrangement - Pinacol-pinacolone rearrangement, Dieone-phenol rearrangement, Benzil-benzilic acid rearrangement, Wolff rearrangement, Tiemann rearrangement, The Arndt-Eister synthesis, The Baeyer -Villiger rearrangement, The Wittig Rearrangement, The Wallach rearrangement. **(7 hrs)**

Module IV

Elimination reactions: Beta Elimination, Alpha elimination, Cis eliminations, Discussion of E1, E2, E1CB Mechanism and orientation. Orientation of the double bond, Saytzeff and Hoffmann rules. Stereochemistry of E2 reactions. Pyrolytic eliminations, Stereochemistry of syn- elimination, Cleavage of quarternary ammonium hydroxides, Eliminations Vs substitutions.
Reaction formation of Carbon-carbon and carbon-heteroatom multiple bonds - Shapiro reaction, Peterson reaction, Julia reaction, deoxygenation of *vic*-diol, Ramberg-Backlund reaction, Dehalogenation of vicinal dihalides, Nitrile formation, fragmentation, Extrusion reaction. **(10 hrs)**

Module V

Addition reactions: Addition to multiple bonds, eletrophilic addition mechanism, Markownikoff's rule, Khrasch effect, Nucleophilic mechanism, Addition to diene, Free radical mechanism, Cyclic mechanism (Diels-Alder reaction), Addition to C-C double and C-C triple bond - halogenations, addition of amine, ene reaction, Michael reaction, 1,4-addition, alkylation, acylation, reaction with OsO_4, and $KMnO_4$, Prevost reaction, 1,3-dipolar addition,
Addition to C-O double bond - Formation of acetal and ketal, formation of dithiane, Formation of imine and enamine, Stork enamination reaction, Mannich reaction, Grignard reaction, Reformatsky Reimer-Tiemann reaction, reaction with active methylene group (Knoevenagel and Stobbe reactions), Claisen condensation, Darzen reaction, Benzoin condensation, Strecker synthesis, Prins reaction, Reactions with phosphorous ylides and sulfur ylides (overview).

Addition to C-N double and C-N triple bond - hydrolysis (acid or base catalysis), addition to amine, Thorpe reaction, Ritter reaction. Addition to C-S double bond - Reaction with amine. **(10 hrs)**

Texts Books / Reference Books:

1. Advanced Organic Chemistry – J. March, Wiley Interscience.
2. Mechanism and Structure in Organic Chemistry – E. S. Gould (Holt, Rinehart and Winston)
3. A Guidebook to Mechanism in Organic Chemistry – Peter Sykes
4. Organic Chemistry – J.Clayden; N.Greeves; S. Warren; P. Wothers

Computer Fundamentals and Programming
Subject Code: CH20107A (with effect from January 2023)

Credit 4 **Contact hours:** 4 hrs/week

Objectives: The first part of the course aims to introduce students to the fundamentals of Computers and computing and imbibe virtues of proper computing techniques. The second part of the course deals with writing programs in C. The course progresses with increasing level of difficulty and complexity of C-programs. Use of loops, OR, AND and NOT operators, Arrays and finally functions and sub-programs in programs are included.

Course Outcome:
CO1: Understand the functioning of functioning of hardware and software.
CO2: Knowledge of basics of C-programming.
CO3: Ability to write C-programs using conditional statements and loops.
CO4: Ability to write C-programs for solving common analytical problems in chemistry.

Module –I

Computer Fundamentals: Introduction, Hardware and software, programming languages and translators Concepts of algorithm and flowcharts.
Computation: Introduction to number systems: binary, octal, decimal and hexadecimal, representation of numbers: Integer and floating point representation, word length, overflow and underflow
Significant digits, accuracy and precision, approximations and errors in computing, machine epsilon, minimizing the total error, pitfalls and precautions during computation. **(8hrs)**

Module –II

Types of Constants in C, syntax rules, identifiers and keywords, data types declaring variables, defining constants and pre-processor directives.
Operators & Expressions: Unary, Arithmetic, relational and logical operators, increment and decrement operators, precedence & associativity operators.
Input and Output: Standard and formatted input-output. **(8hrs)**

Module –III

Conditional statements, switch. **Loops**: *for, while and do while*, break and continue with at least 1 illustrative program each. **(8hrs)**

Module –IV

Functions and Sub-programs: Importance and advantages of sub-programs, defining and calling function, global, local and static variables. **(8hrs)**

Module –V

Arrays: One dimensional and multidimensional array, reading and writing multidimensional arrays, addition, subtraction, multiplication and other operations with matrix.

Application of C Programming to Chemistry related problems, use of numerical methods. **(8hrs)**

Texts Books / Reference Books:

1. Computer programming in C. – V. Rajaraman
2. Programming in ‘C’ – Balguruswamy
3. Programming with ‘C’ – Byron S. Gottfried
4. Numerical Methods – E. Balaguruswamy

Quantum Chemistry- I
Subject Code: CH20108A (with effect from January 2023)

Credit 3 **Contact hours:** 4 hrs/week

Objectives: The course aims to introduce students to the fundamental principles of Quantum Chemistry and its application to some model systems and their modified forms to real systems, specially the hydrogen atom.

Course Outcome:
CO1: To acquire basic knowledge in fundamentals of quantum chemistry.
CO2: To understand the concept of wave function through the Schrodinger equation and understand the use of operators in quantum mechanics.
CO3: To understand the applications of Schrodinger equation in simple systems like atoms and molecules.
CO4: To acquire knowledge on quantum mechanical treatment of the Harmonic Oscillator, Energy eigenvalues and symmetry of the wave function.
CO5: To understand the use of Schrodinger wave equation in polar co-ordinates, particle in a ring, angular momentum and particle on a sphere model.

Module I

Introduction to wave mechanics; Black Body radiation, Planks Quantum theory, Photoelectric Effect, Compton Effect, De Broglie's Theory of matter waves, Derivation of de Broglie's equation; Bohr's principle from de Broglie's relationship; Consequences & limitation of de Broglie's equation; Experimental verifications; Heisenberg's uncertainty principle, Mathematical expression for Uncertainty principle; Experimental verification of Uncertainty principle; Outcome, limitations & applications of uncertainty principle. **(10hrs)**

Module II

Schrödinger's wave equation and its derivation, physical significance of ψ and ψ^2, condition of normalization and orthogonality, quantum mechanical operators and their algebra and properties, Eigen value and Eigen functions, the four basic postulates of quantum mechanics, Schrödinger's wave equation with respect to time; Physical significance of ψ; Postulates of quantum mechanics. **(10hrs)**

Module III

Wave function of a free particle system, particle in a one-dimensional box and its application to a linear conjugated hydrocarbon like butadiene system, derivation of Schrödinger equation for a particle in a three-dimensional box, Wave mechanical treatment of a particle in a cubical box: Degeneracy of energy levels, symmetry of wave functions. **(10 hrs)**

Module IV

Harmonic Oscillator: Classical treatment of a HO and its graphical representation. Energy conservation in HO. Quantum mechanical treatment of the HO, Energy eigenvalues, symmetry of the wave function. Hermite Polynomials in HO. (**5 hrs)**

Module V

Schrodinger wave equation in polar co-ordinates, particle in a ring, angular momentum, Particle on a sphere, l and M quantum numbers, space quantization of angular momentum, spherical harmonics in real form. Application to rotation of a diatomic molecule plane and in space. Wave mechanical treatment of hydrogen atom. **(5hrs)**

Reference Books:

1. R.K.Prasad," Quantum Chemistry", New Age International Publishers.
2. Chandra, A. K. Introductory Quantum Chemistry Tata McGraw-Hill (2001).
3. House, J. E. Fundamentals of Quantum Chemistry 2 nd Ed. Elsevier: USA (2004). • Lowe, J. P. & Peterson, K. Quantum Chemistry, Academic Press (2005).
4. Ira.N. Levine, Quantum Chemistry, 5th edition (2000), Pearson educ., Inc.New Delhi
5. McQuarrie, D. A. Quantum Chemistry Viva Books Pvt Ltd.: New Delhi (2003).

Computer Programming Lab
Subject Code: CH20403A

Credit: 3 **Contact hours:** 6 hrs/week

Objectives: To enable the students to write and execute simple as well as complex computational programs and apply them to chemistry related problems.

Course Outcome:
CO1: Ability to write simple programs using logical operators, loops and arrays.
CO2: Simplify complex problems using functions.
CO3: Ability to write C-programs for data analysis for chemical problems.

1) Familiarization and introduction of computers, editors.
2) Simple Programs:
To find simple & compound interest, factorial.
Conversion of binary to decimal numbers, octal, hexadecimal.

Evolution of series
Solving some simple problems related with chemistry.
3) Problems based on understanding of various statements, if-else statements, loops like *for, while*, etc
4) Problems related to arrays and matrices.
5) Functions: Programs involving calling a sub-program.

Texts Books / Reference Books:
1. Computer programming in C. V. Rajaraman
2. Programming in 'C', Balguruswamy
3. Programming with 'C', Byron S. Gottfried
4. Numerical Methods E. Balaguruswamy

Organic Chemistry Lab
Subject Code: CH20404A

Credit: 3 **Contact hours:** 6 hrs/week

Objective: To make them aware on the various techniques adopted in organic synthesis. And also accustom them about modern methods used in various biologically important organic molecules.

Course Outcome:
CO1: Learn and apply techniques used in Organic Chemistry laboratory for synthesis, purification and identification.
CO2: Employ the basic techniques used in Organic Chemistry laboratory for analysis such as chromatography, spectroscopy and estimation.

1. Demonstration of simple distillation, distillation under reduced pressure, thin layer chromatography (TLC) / PTLC, crystallization and Columnn chromatography.
2. Estimation of Glucose and phenol or acetone
3. Organic synthesis: (Introduction of Green organic synthesis)
   (a) Bromination
   (b) Acetylation
   (c) Nitration
   (d) Some name reactions
4. Organic synthesis with solid support. (with or without microwave irradiation)

Texts Books / Reference Books:
1. Vogel's text book of practical organic chemistry - Furniss Hannaford Smith, Tatchell
2. Monograph on Green Chemistry – Laboratory Experiment - Green Chemistry task force committee, DS

Advanced Coordination Chemistry & Inorganic Reaction Mechanism
Subject Code: CH20109A (with effect from August 2022)

Credit 4 **Contact hours:** 4 hrs/week

Objectives: Detailed understanding of CFT, MOT and their use in inorganic complexes. Understanding of various types of transitions and their interpretation. Introduction to reaction mechanism with examples.

Course Outcome:
CO1: Understanding of VBT, CFT and their applications.
CO2: Ability to predict electronic transitions and interpret electronic spectra of transition metal complexes and influence of distortion.
CO3: Understanding fundamentals of molecular orbital theory.
CO4: Understanding fundamentals of reaction mechanism & electron transfer reaction mechanism.
CO5: Understand the importance of use of organometallic catalysts in different reactions & bonding in carbonyl complexes

Module I

Nature of metal ligand Bonding in complex compounds:

Valence bond theory in octahedral, tetrahedral & square planner complexes Crystal Field Theory – Crystal field theory (CFT) – Splitting of d orbital in octahedral, Tetrahedral and square planner complex, factors influence the magnitude of Δ_o, application of CFT. **(8hrs)**

Module II

Crystal Field Stabilization Energy (CFSE)
Determination of Δ_o (CFSE) for various configurations. Microstate table and its use in predicting electronic transitions. Jahn-Teller Distortion**.**
(8 hrs)

Module III

Molecular Orbital Theory (MOT)
Molecular Orbital Theory (MOT), MOT in octahedral complexes, Energy order of orbitals and their filling with electrons, π bonding in octahedral complexes. Electronic spectra of complexes. **(8 hrs)**

Module IV

Inorganic reaction mechanism:
Substitution and electron transfer reaction - Nucleophilic Substitution in square planar and octahedral complexes, Kinetics, Associative- Dissociative mechanisms, Trans effect, influence of acids-bases and other factors in reactions. Outer sphere and Inner sphere electron transfer, Sq. planar and octahedral complexes, excited state electron transfer and its application. **(8 hrs)**

Module V

Special organometallics & Bonding in Carbonyl complexes:
Bonding in Carbonyl complexes, Special organometallics - Reaction and applications, Suzuki reactions, Stille reaction, Negishi Cross coupling, Heck reactions, Buchwald-Hartwig Reaction, Sonogashira reactions. **(8 hrs)**

Texts Books / Reference Books:

1. Advanced Inorganic chemistry - F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochman
2. Inorganic Chemistry, Principles of Structure and Reactivity - James E. Huheey, Ellen A. Keiter, Richard L. Keiter
3. Inorganic Chemistry - Atkins and Shriver
4. Inorganic Chemistry – G. L. Miessler, P. J. Fischer & D. A. Tarr

Concepts in Organic Synthesis
Subject Code: CH20110A (with effect from August 2022)

Credit 4 **Contact hours:** 4 hrs/week

Objective: This course will introduce the basic idea of Pericyclic reactions, Organic photochemistry, concepts of oxidation-reduction, heterocyclic chemistry and introduction of natural products.

Course Outcome:
CO1: Ability to identify and deduce mechanisms of various types of pericyclic and photochemical reactions.
CO2: In-depth understanding of solid state chemistry of peptides and its applications.
CO3: In-depth understanding of catalysis in chemistry and its applications.
CO4: Ability to identify and apply the oxidation-reduction reactions in synthesis.
CO5: In-depth knowledge of heterocyclic chemistry and its applications.

Module - I

Pericyclic Reactions
Pericyclic reactions: conservation of molecules orbital symmetry, Introductory FMO theory, Electrocyclic reactions-conrotatory and disrotatory approach, stereochemistry, Cycloaddition reactions - Diels-Alder (mechanism, regioselectivity, stereochemistry), catalyzed Diels-Alder reaction, asymmetric Diels-Alder reaction, retro Diels-Alder reaction, [2+2]-cycloaddition, ene reaction (in details). Sigmatropic rearrangement - [3,3]-sigmatropic (cope, aza-cope, anionic oxy-cope, Claisen, aza-Claisen rearrangement) rearrangements, mechanism and stereochemistry, [2,3]-sigmatropic rearrangements, aza-Wittig rearrangement, Sommelet-Hauser rearrangement, [2,3]-Meisenheimer rearrangement. Cheletropic group transfer reactions. Synthetic of bioactive molecules using pericyclic reaction. **(9 Hrs)**

Module - II

Organic Photochemistry
Principle, photochemical energy, orbital symmetry consideration related photochemical reactions, electronic oxidation, excited state of organic molecule, modes of dissipation of energy, energy transfer, quantum yield, cis-trans isomerization, photo-fragmentation reaction (Barton, Hofmann-Loffler-Freytag), Norrish type (I) & (II) reactions, Paterno Buchi reaction, Photo reduction, di-pi methane, aza-di-pi methane rearrangement, photocyclo addition, Photo chemistry of α, β- unsaturated ketones, reaction with singlet oxygen, application of photochemical methods in organic synthesis (Tranylcypromine). **(8 Hrs)**

Module - III

Oxidation & Reduction Reaction
Reduction: Reduction of C-C multiple bond and carbon-hetero multiple bond: Catalytic hydrogenation (both hydrogen and hydride transfer mechanism), Electrochemical reduction at a low overvoltage electrode, Reduction by metal hydrides and alkoxides (LAH, DIBAL-H, Bu_3SnH), Borane and borohydride, R_3SiH, Reduction by dissolving metals, Stereo/enantioselectivity reductions (Chiral Boranes, Corey-Bakshi-Shibata).
Oxidation: Formation of C=C by dehydrogenation – dehydrogenation by selenium dioxide, Formation of alcohols from hydrocarbons, Jones reagent, Sarett's reagent, PCC, Swern oxidation, MnO_2, IBX, MPV, $Pb(OAc)_4$, $NaIO_4$, HIO_4, Dakin reaction, O_3, *m*-CPBA, $VO(acac)_2$, Sharpless asymmetric epoxidation. **(7 Hrs)**

Module - IV

Heterocyclic Chemistry
Introduction, classification, nomenclature, reactions of azeridine, oxirane, thiirane, oxaziridine, azetidine, azetidinone, oxetane, oxetanone, thietane, pyrrole, furan, thiophene, 1,2- and 1,3-azoles, triazoles, pyridine, diazines, triazine and their oxy-derivatives. Application of heterocycles in various emerging field - especially in medicine, and natural products. **(7 Hrs)**

Module - V

Catalysis
Heterogeneous catalysis: Preparation of catalyst and applications heterogeneous catalysis in synthesis of drugs. Homogenous catalysis: Introduction, hydrogenation, Wilkinson catalysts, Ziegler-Natta catalysts, applications of homogeneous catalysis in synthesis of drugs. **(6 Hrs)**

Chemistry of Peptides
Principle and methods of solid phase peptide synthesis, activation procedures, coupling reactions, protection, deprotection and cleavage from resin. **(3 Hrs)**

Texts Books / Reference Books:

1. Finar, I. L., Organic Chemistry, vol. I & II (ELBS).
2. Advanced Organic Chemistry by J. March, Wiley Interscience.
3. Organic Chemistry by Morrison and Boyd
4. Reaction mechanism in organic chemistry by Mukhreji & singh
5. Design of organic synthesis by M.Taylor
6. Stereochemistry of Carbon Compounds – E. L. Eliel
7. Organic Chemistry – J. Clayden; N. Greeves; S. Warren; P. Wothers
8. Modern Methods in Organic Synthesis – W. Carruthers

Chemical Dynamics and Electrochemistry
Subject Code: CH20111A (with effect from August 2022)

Credit 4 **Contact hours:** 4 hrs/week

Objective: The objective behind studying Chemical dynamics and electrochemistry is to present theories and applications related to the various chemical reactions and also to update the students with the latest developments in the above field.

Course Outcome:
CO1: To impart basic knowledge of Chemical Kinetics of Collision theory and the activated complex theory. To understand the mechanisms of unimolecular reactions.
CO2: To understand the chemistry of Complex reactions, consecutive reactions, chain reactions, oscillatory, Thermal & photochemical chain reactions. To understand the kinetics of fast reactions.
CO3: To acquire knowledge on the principles of Debye-Huckel model of ion-ion interactions and its verification.
CO4: To understand the theory of electrolytic conductance and the principle of Dispersion of conductance through the Debye- Falkenhagen effect and Wien effect.
CO5: To impart knowledge on the chemistry of Ion-Solvent interaction, its concept, the experimental determination and its application to equilibria.

Module I

Chemical Kinetics-I: Arrhenius equations, concept of transition state, transition state theory-mechanism, collision theory, steric factor, comparison between collision & Transition state theory, Potential energy surface, thermodynamic treatment of reaction rates, Energy of activation, volume of activation, Series & Parallel reactions, Equilibrium from kinetic point of view, Kinetic isotope effect and solvent isotope effect, treatment of unimolecular reactions-Lindemann's theory , Hinshelwood's theory. **(12hrs)**

Module II

Chemical Kinetics-II: Complex reactions, consecutive reactions, chain reactions and oscillatory, Thermal & photochemical chain reaction between H_2 & Cl_2 and H_2 & Br_2, Influence of dielectric constant and ionic strength on reaction rate, linear free energy relationship, effect of substituents, fast reactions. Luminescence and energy transfer process, study by stop flow techniques, relaxation method. **(10hrs)**

Module III

Electrochemistry- Ideal & nonideal solutions, activity & activity coefficients, its method of determination, Onsager equation, Debye – Huckel theory of dilute electrolytes, derivation of Debye-Huckel conductance equations for dilute solution, Verification of Debye – Huckel theory. **(8hrs)**

Module IV

Limiting & extended Debye-Huckel equation for activity coefficient, osmotic coefficient, test of the theory. Theory of electrolytic conductance: Degree of dissociation, time of relaxation, Mechanism of electrolytic conductance. Dispersion of conductance: Debye- Falkenhagen effect and Wien effect. Huckel- Bronsted effect. **(4hrs)**

Module V

Ion-Solvent interaction, concept, experimental determination, application to equilibria, kinetics, universal scales of potential acidity & basicity in different solvents, Theories, Born model & Eley-Evans model, Absolute heat of hydration (Halliwel & Nyburg method), Solvation number & its determination, ion-solvent, nonelectrolyte interaction, salting out & salting in phenomena. **(6hrs)**

Reference Books:

1. Laidler, K. J. Chemical Kinetics 3rd Ed., Pearsons (2011).
2. Atkins, P. W. & Paula, J. de Atkin's Physical Chemistry 8th Ed., Oxford University Press (2006).
3. McQuarrie, D. A. & Simon, J. D. Physical Chemistry: A Molecular Approach 3rd Ed., Univ. Science Books (2001).
4. Bockris, J. O' M. & Reddy, A. K. N. Modern Electrochemistry 1: Ionics 2nd Ed., Springer (1998).
5. Bockris, J. O' M. & Reddy, A. K. N. Modern Electrochemistry 2B: Electrodics in Chemistry, Engineering, Biology and Environmental Science 2nd Ed., Springer (2001).
6. Bockris, J. O' M., Reddy, A. K. N. & Gamboa-Aldeco, M. E. Modern Electrochemistry 2A: Fundamentals of Electrodics 2nd Ed., Springer (2001).
7. Brett, C. M. A. & Brett, A. M. O. Electrochemistry, Oxford University Press (1993).
8. Moore, W. J. Physical Chemistry 4th Ed. Prentice-Hall (1972).
9. Electrochemistry, S. Glasstone.

Biochemistry
Subject Code: CH20112A (with effect from August 2022)

Credit 4 **Contact hours:** 4 hrs/week

Objective of Biochemistry paper is to introduce the chemical nature of biomolecules and various types of biochemical reactions involved in chemistry of life. Biochemistry is a well-established exciting discipline, and a very promising research area for M.Sc. Chemistry pass outs.

Course Outcome:
CO1: Basic knowledge of biomolecules, biochemical solvents, important functional groups, importance of non-covalent bonds in biochemistry and biochemical thermodynamics
CO2: Fundamental knowledge of protein, carbohydrate and lipid structures and functions
CO3: Basic knowledge of polynucleotide structures, gene, genetic code, protein synthesis within cell and control of genetic expressions
CO4: Fundamental knowledge about the relationship between properties and structure of the enzymes, their mechanism of action and kinetics of enzymatic reactions.
CO5: An understanding of biochemistry in photosynthesis, carbon assimilation, functioning of the biochemical components of photosystems, photoexcitation and de-excitation of LHC.

Module I

Introduction to Biochemistry: **(8Hrs)**
Functional groups of biochemical importance (1hr)
Water as a biochemical solvent, unique physico-chemical properties of water, importance of hydrogen bond in water and biomolecules (2hrs),
Biochemical evolution of life(1hr)
How do cells use energy? – connection between metabolic reactions and energy (1hr)
Spontaneity in biochemical reactions –connections thermodynamics and life (1hr)
Biochemical aspects of cellular structure (1 hr)
Microscopy in biochemistry – standard light microscope, scanning and transmission electron microscopes – SEM & TEM (1hr)

Module II

Protein: (**7Hrs**)
Basic structure of amino acids, stereoisomerism, classification of 20 essential amino acids (1 hr)
Peptide bond and primary structure of protein (1hr) Alpha helix and beta pleated sheet structure of protein (secondary structure) (1hr)
Supramolecular structure of collagen triple helix with functional importance (1 hr)
Tertiary structure of protein with special reference to myoglobin, important non-covalent and hydrophobic interactions in tertiary structures (1 hr)
Application of XRD and NMR techniques to delineate tertiary structures (1hr)
Quaternary structures of protein (1hr)

Module III

Carbohydrate and Lipid: **(5Hrs)**
Carbohydrate – Monosaccharide, disaccharide and polysaccharide (1hr)
Lipid metabolism – Fatty acids, fatty acid breakdown, properties and functions of triglycerides, phospholipids and glycolipids (4hr)

Module IV

Enzymes: **(10Hrs)**
General characteristics and the role of enzymes, holoenzyme, apoenzyme, coenzymes, prosthetic groups (2h).
Factors affecting enzyme activity- pH, temperature, enzyme and substrate concentrations (2h).
Michaelis-Menten equation for unimolecular reaction, Reaction rates for multistep reactions, the significance of K_M K_{cat} and V_{max} (2h).
Reversible and irreversible inhibition; competitive, non-competitive and uncompetitive inhibitions with determination of K_M and V_{max}(2h).
Allosteric enzymes, Cooperativity, concerted and sequential models (2h).

Module V

Photosynthesis: **(10Hrs)**
The basic processes of photosynthesis, quantum yield and quantum efficiency (2h).

Photosynthetic electron transport and generation of NADPH & ATP, Photosystems I and II, their location, the light reactions mechanism of quantum capture and energy transfer in Photosystems, cyclic and noncyclic photoinduced electron flow (4h). The dark reactions: The Calvin cycles (2h),
The Hill reaction and photophosphorylation, reduction of carbon dioxide: C3, C4 and CAM metabolism with regulation (light activation of enzymes in them) (2h).

Texts Books / Reference Books:

1. Biochemistry – Lehninger
2. Instant Notes in Biochemistry – B D Hames, N M Hooper & J D Houghton Viva Books Private Limited
3. Biochemistry – Mathews & Holde Pearson Education
4. Biochemistry – Campbell & Farrell Thompson
5. Biological Science by Taylor & Green Cambridge University Press
6. Biochemistry – Rastogi Tata McGrawHill
7. Modern Biotechnology – S B Primrose Blackwell Scientific Publication

Photoinorganic Chemistry
Subject Code: CH20301A (with effect from August 2022)

Credit 4 **Contact hours:** 4 hrs/week

Objective- Introduction to photochemistry, concepts, application and industrial use.

Course Outcome:
CO1: In- depth understanding of photochemical Laws, Ability to explain various photophysical process taking place in excited state and factors influencing them.
CO2: Ability to identify and explain photophysical kinetics of excited state in gaseous and liquid state and electron transfer process
CO3: In-depth understanding of photo-reduction and related reactions.
CO4: Ability to identify various types of photochemical reactions and its application.
CO5: In-depth understanding of photochemical reactions in biological processes and its explanation using model systems.

Module I

Introduction to inorganic photochemistry:
Introduction to inorganic photochemistry, Photophysical process in electronically excited molecules - Jablonski diagram, radiationless transitions, selection rules. Fluorescence emission, fluorescence and structure.
Triplet states and phosphorescence emission, photophysical kinetics of unimolecular process, delayed fluorescence, effect of temperature.
Photophysical kinetics of bimolecular process – kinetic and optical collisions, collision in gases and vapours**.**
(8Hrs)

Module II

Collisions in solution & kinetics
Collisions in solution, kinetics – of quenching, Stern-Volmer equation, deviations
Excimer and excited state dimers, exciplex formation and decay.
Long range and short range electron transfer, intramolecular energy transfer, exciton transfer, liquid scintillators.
(8Hrs)

Module III

Photo Reduction and Related Reactions
Photo reduction and related reactions, Photo oxidation and photo oxygenation, Chemiluminescence, Photosensitization. Photochemical reactions; substitution, decomposition and fragmentation, rearrangement, and redox reactions. **(8Hrs)**

Module IV

Photochemical Reaction
Photochemical reaction between anthrance and carbon tetrachloride, determinations of quantum yields of reaction, Reaction of anthracene with other halogenated solvents, Photoreactive state of anthracene. **(8Hrs)**

Module V

Selective Inorganic Photochemistry
Selective inorganic photochemistry using laser beams. Inorganic photochemistry in biological processes and their model studies- Mutagenic effect of radiation, Photosynthesis. **(8Hrs)**

Texts Books / Reference Books:

1. Organometallic Photochemistry, Academic Press, 1979 – G.L. Geoffrey & M.S. Wrighton
2. Fundamentals of Photochemistry, Wiley Eastern, 1978 – K.K. Rohatagi-Mukherjee
3. Inorganic and Organometallic photochemistry, ACS Pub., 1978 – M.S. Wrifhron
4. Photochemistry of Co-ordination compounds, Academic Press, 1970 – V. Balzani and V. Carasiti

Synthetic Organic Chemistry
Subject Code: CH20302A (with effect from August 2022)

Credit 4 **Contact hours:** 4 hrs/week

Objective: This course will discuss the use of various organometallic compounds in organic synthesis, chemistry of B, Si, P, S and Sn. Moreover, the role of transition metal complexes in organic synthesis and asymmetric synthesis will be covered in this subject area. Knowledge on retrosynthesis, protection & deprotection of functional group and application of spectroscopy for the determination of organic structures will be provided to make clear understanding among students about the organic synthesis.

Course Outcome:
CO1: A comprehensive knowledge of organometallic and their uses in organic synthesis.
CO2: A comprehensive knowledge of organometalloid and their uses in organic synthesis.
CO3: Ability to demonstrate knowledge of asymmetric synthesis.
CO4: Ability to design retro-synthetic strategies independently for compounds of moderate complexity.
CO5: Ability to project and deprotect functional group during organic synthesis.

Module I

Organometallic compounds of Group I and II metals in organic synthesis and B, Si, P, S, Sn chemistry.
Organomettalic compound of Gr I and II metals: preparation and properties, reaction with carbonyl and alkylating agents.
Boron Chemistry: Organoboranes- preparation and properties of organoborane reagents e.g. RBH_2, R_2BH, R_3B, 9-BBN, Thexyl borane, cyclohexyl borane, Hydroboration-mechanism, stereo and regioselectivity, uses in synthesis of primary, secondary tertiary alcohols, aldehydes, ketones, alkenes. Synthesis of E, E; E, Z; Z, Z dienes and alkynes. Allyl boranes- synthesis, mechanism and uses.
Phosphorous chemistry: preparation & properties of PPh_3, $P(OEt)_3$, $POCl_3$, PBr_3, PCl_5, etc. Wittig-Horner reaction, Mitsunobu reaction, Staundinger reaction, Vilsmeier-Haack reaction, Corey-Winter reaction.
Silicon chemistry: reaction with TMSCl, *i*-Pr_3SiCl in organic synthesis.
Sulphur chemistry: reaction with CS_2, SO_2, SO_3, $SOCl_2$, SO_2Cl_2, PhSNa, 1,3-dithiane, DMSO, RSCl, sulphur ylide in organic synthesis.
Tin chemistry: synthesis of organostannanes, carbon-carbon bond forming reaction with organostannanes.
(12 Hrs)

Module II

Transitional metals complexes in organic synthesis
Introduction, oxidation states of transition metals, 16-18 rule, dissociation, association, insertion, oxidative addition, reductive elimination of transition metal
Organocopper intermediates: preparation and structure, reaction involving organocopper.
Organopalladium in organic synthesis- Heck arylation, allylic activation, carbonylation, wacker oxidation, isomerization formation N-aryl and N-alkyl bond transmetalation, allyl deprotection in peptides.
Organo nickels- coupling carboxylation, carbonylation. Reaction involving rhodium and ruthenium. **(8 Hrs)**

Module III

Asymmetric synthesis
Asymmetric synthesis: stereoselective and stereospecific reactions, prochirality, Chemo-, regio-, diastereo- and enantio-controlled approaches; Chirality transfer, Asymmetric inductions; Chiral pools, Chiral auxiliaries, Chiral reagents and catalysts, and templates;
Asymmetric oxidations: dihydroxylation, aminohydroxylation, Asymmetric reduction reactions: Reduction of ketones, imines and olefins (use of BINAP)
Asymmetric C-C bond forming reaction: Simmon-Smith reaction, Mukaiyama aldol reaction, Shibasaki bi-metallic catalyst system; Meyers oxazoline and bis-lactam based methods; Henry reaction, Baylis-Hillman-Morita reactions, Asymmetric allylation, Asymmetric hydroformylation. **(10 Hrs)**

Module IV

Retrosynthesis

Retrosynthesis analysis: Basic principles and terminology of retrosynthesis, one group and two group C-X disconnections, one group C-C and two group C-C disconnections, amine and alkene synthesis, important strategies of retrosynthesis, functional group transposition, important functional group interconversions. **(5 Hrs)**

Module V

Protection & Deprotection of functional group

Protecting groups: Protection and deprotection of hydroxy, carboxyl, carbonyl, carboxy amino groups and carbon-carbon multiple bonds; chemo- and regioselective protection and deprotection; illustration of protection and deprotection in synthesis. **(5 Hrs)**

Texts Books / Reference Books:

1. Advanced Organic Chemistry by J. March, Wiley Interscience.
2. Organic Chemistry by J.Clayden; N.Greeves; S. Warren; P. Wothers
3. Principles of Organic Synthesis by R.O.C. Norman
4. Modern methods in organic synthesis Organic Synthesis by W. Carruthers and I.Coldhalm
5. Advanced Organic Chemistry - Part B: Reactions & Synthesis by F.A.Carey & R.J.Sundberg
6. Chiron approach in organic synthesis by S. Hanessian (Relavent chapters for Chirons)
7. Asymmetric Reactions and Processes in Chemistry: Ernest L. Eliel
8. Comprehensive Organic Transformations: A Guide to Functional Group Preparations, 2nd edition (1999) by Richard C. Larock.
9. Protective Groups in Organic Synthesis, 3rd edition (1999) by Theodora W. Greene and Peter G. M. Wuts

Advanced Physical Chemistry
Subject Code: CH20303A (with effect from August 2022)

Credit 4 **Contact hours:** 4 hrs/week

Objective: To introduce the concepts of statistical mechanics and thermodynamics as it relates the macroscopic properties of a system to the properties of the atoms and molecules which constitutes a system.

Course Outcome:
CO1: Able to find the connection between statistics and thermodynamics. and differentiate between classical statistics and quantum statistics
CO2: Able to account for the physical interpretation of partition functions and be able to calculate thermodynamic properties of model systems with using Boltzmann, Fermi-Dirac and Bose-Einstein statistics.
CO3: Able to understand process of aggregation of amphiphilic molecules and their industrial application.

Module I

Basic Statistical Thermodynamic, Phase space, Assembly & Ensemble, canonical form, statistical equilibrium & thermodynamic probability, Maxwell Boltzmann statistics. **(5Hrs)**

Module II

Partition function and its types – Translational, Rotational, Vibrational, and Electronic partition function. Relations of partition function with thermodynamic functions such as internal energy, heat capacity, Entropy & probability, heat content, work function 'A', Gibb's free energy, heat content and third law of thermodynamics and equilibrium constant from partition functions. **(10Hrs)**

Module III

Quantum Statistics- Bose- Einstein & Fermi Dirac statistics, Theories of specific heat of solids -Einstein and Debye treatment. **(5Hrs)**

Module IV

Surfactants and interfacial Phenomena:
Introduction: Characteristic features of surfactants and amphiphiles. Various types of amphiphiles. Self-assembly and the critical packing parameter. Factors affecting self-aggregation. **(10Hrs)**

Module V

Experimental methods for detection of self-aggregation. Thermodynamic parameters of amphiphilic aggregation. Vesicles, Types of vesicles, Gel-to-liquid crystalline phase transition. Differential Scanning Calorimetey studies. Litchenberg three stage model. **(10Hrs)**

Texts Books / Reference Books:

1. Surfactants and Interfacial Phenomena– Milton J. Rosen. John Wiley & Sons, Inc
2. Surfactant Aggregation– J.H. Client. Springer
3. Thermodynamics-A core course – Srivastava, Saha & Jain.
4. Statistical Thermodynamics – M.C.Gupta
5. Fundamentals of classical and Statistical Thermodynamics-B.N.Roy
6. Classical and Statistical Thermodynamics- A.H.Carter

Inorganic Chemistry Lab
Subject Code: CH20405A – No modification

Credit: 3 **Contact hours:** 6 hrs/week

Objective: To gain experience in synthetic techniques and interpretation of the spectras on the basis of concepts learned in theory.

Course Outcome:
CO1: Ability to synthesize different first row transition metal complexes, their purification and crystallization.
CO2: Ability to determine percentage of yield of the products and to characterize physical properties.
CO3: Ability to carry out UV-vis spectroscopic studies of the prepared complexes.
CO4: Ability to analyse UV-vis spectral data (Molar extinction coefficient, identification of d-d transistion and charge transfer).

List of Experiment

1. Synthesis of first row transition metal complexes and their purification (minimum of 10 complexes).
2. UV-vis spectroscopic studies of the prepared complexes:
   a) Role of metal ions
   b) Influence of ligands
   c) Total interpretation of spectra and correlation with CFT

Texts Books / Reference Books:
1. Co-ordination Chemistry Reviews
2. Journal of Chemical Education
3. Inorganic Chemistry, Principles of Structure and Reactivity – James E. Huheey, Ellen A. Keiter, Richard L. Keiter

Bio-inorganic Chemistry
Subject Code: CH20113A (with effect from January 2023)

Credit 4 **Contact hours:** 4 hrs/week

Objective: The students will acquire in-depth knowledge of role of transition metal ions and its complexes in different biological processes and their chemistry in treatment of different diseases

Course Outcome:
CO1: Understanding of basic reactions in the biological systems and storage & transport of metabolic energy.
CO2: Ability to understand ion transport across the biological membrane.
CO3: In-depth knowledge of biological redox reactions, their importance and dioxygen in biological systems.
CO4: In-depth Knowledge of metalloproteins in biological system and their active site structures.
CO5: Knowledge of metalloenzymes and their applications in biological systems.

Module I

Basic Biological Inorganic Reaction:
a) Basic reactions in the biological system and the roles of metal ions. Metal complexes in medicine- cisplatin, auranofin, Replication, Transcription & Translation of DNA**.**
b) Metal – nucleic acid interactions - Metal ion interaction with Nucleosides & Nucleotides, Metal ion interaction with DNA, Metal ion interaction with RNA.
c) ATP =ADP Interconversion, Creatine- Phosphocreatine interconversion, phosphate transfer and its activation by metal ions. (**8Hrs)**

Module II

Transport Across Biological Membrane:
Transport Across Biological membrane – Ionophores as metal ion carriers- cyclic natural ionophores, open chain carboxylic acid ionophores & other ionophores. Active transport across the membrane.
Na^+/K^+ transporting AT Pase, Na^+ ion pump**.** **(8Hrs)**

Module III

Biological Redox Reaction: Biological Redox Reaction- Electron transport proteins – Ferredoxins, Cytochromes. Energetics of electron transport in the respiratory chain.
Photosynthesis & chlorophyll
Dioxygen in Biological system- Reactions of molecular oxygen, Activation of Dioxygen Molecule in Transition metal Dioxygen complexes. **(8Hrs)**

Module IV

Metalloproteins:
Oxygen carrying proteins- Haemoglobin & Myoglobin, Hemerythrin, Hemocyanin, **cooperatively in haemoglobin, bohr effect**, Blood Substitute.
Model system- Synthetic oxygen carriers-
(i) Porphyrin Derivatives,
(ii) Cobalt (II) Dioxygen complexes
(iii) Iridium (II) Dioxygen complexes (Vaska's complexes)
(iv) Platinum group metal dioxygen complexes. **(8Hrs)**

Module V

Metalloenzymes: Redox enzymes- Molybdenum containing enzymes, Iron containing enzymes, Copper containing enzymes, Zinc containing enzymes
Hydrolytic Enzyme-Carboxy peptidase, carbonic anhydrase
Vitamins & co-enzymes.
. **(8Hrs)**

Texts Books / Reference Books:

1. Biochemistry – L. Stryer
2. Principles of Bioinorganic chemistry – S. J. Lippard and J. M. Berg
3. Inorganic Biochemistry – G. L. Eichhorn
4. Elements of Bioinorganic Chemistry – G. N. Mukharjee, A. Das
5. Bioorganic, Bioinorganic and Supramolecular Chemistry – P.S. Kalsi, J. P. Kalsi

Solid State Chemistry & Interface Science
Subject Code: CH20114A (with effect from January 2023)

Credit 4 **Contact hours:** 4 hrs/week

Objectives: The course introduces the concept of molecular arrangements within crystalline solids followed by the aggregation of specific molecules into colloids and its applications.

Course Outcome:
CO1: Able to understand basic concept of crystal structure, its defect and its application to explain electrical properties of the solid material.
CO2: Able to describe the fundamental aspects of colloid and surface chemistry and demonstrate how colloid and surface chemistry is applied in industry and the environment.

Module I

Solid state chemistry: unit cell, Miller indices, Bravais lattice, Bragg's equation, crystal structure analysis, Structure of NaCl, KCl, and Zink Blende, Types of defects in solids and its influence on electrical properties of solids, Insulators & semiconductors and its types, superconductor, band theory. **(16 Hrs)**

Module II

Macromolecules: concept molecular mass, its determination. **(4 Hrs)**

Module III

Surface chemistry: Adsorption of gases on solids, Freundliche's adsorption isotherm, Langmuir adsorption isotherm, Gibb's adsorption equations, BET Application of Adsorption**,** Association colloids:

Module IV

Micelles & reverse micelles micro emulsion formation and thermodynamics application (detergency), Solubilization of surfactant solution Preparation of colloidal sol and application of colloidal Science application , Donnan Membrane equilibrium **(14 Hrs)**

Module V

Photochemistry: Grothoss and Dropess law. Einstein law of Photochemical equivalence, quantum yield, primary and secondary processes, Photoelectric effect, Latent Image, Elementary idea of laser and its application. **(6 Hrs)**

Texts Books / Reference Books:

1. Physical Chemistry of Surface – A.W.Adamson & A.Gast
2. Solid State chemistry and Its Applications-Anthony R. West
3. Basic Solid State Chemistry – A.R.West
4. Solid State Chemstry – Kettal
5. Applied colloid and surface chemistry – R.Pashley
6. Colloids and Interface with Surfactants and Polymer – James W Goodwin

Group Theory – A Chemist Approach
Subject Code: CH20115A (with effect from January 2023)

Credit 4 **Contact hours:** 4 hrs/week

Objective – To provide basic understanding of group theory and its application in chemistry. Exposure to importance of organometallic compounds in industry along with various latest techniques of synthesis.

Course Outcome:
CO1: Ability to identify the symmetry elements and symmetry operation in molecules.
CO2: Ability to identify point group, group multiplication table, subgroups and various groups.
CO3: Ability to make transformation matrix for various symmetry elements.
CO4: Ability to make irreducible character representation of a point group.
CO5: Able to construct character table and apply them to find various properties of molecules.

Module I

Symmetry elements and symmetry operations:
Introduction, importance of symmetry, geometry of molecule through VSEPR theory, different symmetry elements, symmetry operation of each symmetry element, horizontal plane, vertical plane, dihedral plane, associated operation of S_n axis, finding out symmetry elements present in AB_2 (linear and bent), AB_3 (Planar and pyramidal), AB_4 (tetrahedral and planar), AB_5 (planar, triagonal bipyramidal, square pyramidal), AB_6 (planar, octahedral), spiro, unsubstituted and substituted cycloalkane, cyclohexane (chair, boat), conformations of ethane, alkene, alkyne, ferrocene, coronation compounds etc, product of symmetry operations, commutative symmetry operation. **(10 Hrs)**

Module II

Symmetry elements and symmetry operations:
Definition of group, Mathematical rules for the formation of a group, flow chart for determination of point group, symmetry elements present in a point groups, variation of symmetry elements and point group by substitution, order of a group, group multiplication table for a C_s, C_i, C_n, C_{nv}, C_{nh} etc, conjugate elements and classes, subgroup, Isomorphic group, Abelian group, Symmetry number, application of point group on optical activity and dipole moment. **(9 Hrs)**

Module III

Matrix representation of symmetry operation

Definition, order, transpose of a matrix, inverse of a matrix, transformation matrices for i) identity ii) plane of symmetry iii) centre of symmetry iv) axis of symmetry v) improper axis of symmetry. **(6 Hrs)**

Module IV

Representation of point group
Characteristic of matrix representation, character representation of a point group, method for deriving matrix representations on different basis set, method to directly arrive character representation, classification of representations. **(7 Hrs)**

Module V

Character Tables
The great orthogonality theorem, Application of the orthogonality theorem, construction of character tables, Character table of various point group, Mullikan symbols for IR's, Determination of symmetry species for translations and rotations. IR active and Raman active vibrations. **(8 Hrs)**

Texts Books / Reference Books:

1. Chemical Applications of Group Theory – F. A. Cotton
2. Molecular Spectroscopy – D. J. Willock
3. Symmetry and Spectroscopy of Molecules – K. V. Reddy

Quantum Chemistry II
Subject Code: CH20116A (with effect from January 2023)

Credit 4 **Contact hours:** 4 hrs/week

Objectives: The course aims to introduce students to an advanced state of quantum chemistry where the students will apply the basic principles and model systems of quantum mechanics to real systems with the help of approximation methods.

Course Outcome:
CO1: Understanding of approximation methods in quantum chemistry
CO2: Application of these methods for multi-electronic systems
CO3: Application of these methods for explaining chemical bonding.

Module –I

Approximation Methods: Variation method, Linear and nonlinear variation functions and its application in particle in a box, simple harmonic oscillator and hydrogen atom systems. (**8Hrs)**

Module –II

Perturbation Method: First and second order corrections and its application in particle in a box, simple harmonic oscillator and hydrogen atom systems. (**8Hrs)**

Module –III

Application to two electron system.: electron spin, spin orbital, Pauli exclusion rule, columbic and exchange energies. Excited state of He atom, symmetric and antisymmetric wave functions.
Multielectron atoms, determinantal form of the wave function, self-consistent field approximation, Hartree-Fock Self Consistent field theory, Slater type orbitals. (**8Hrs)**

Module –IV

Molecular systems: Separation of electronic and nuclear motions treatment of homonuclear and heteronuclear diatomic molecules- the Born Oppenheimer approximation, MO theory, LCAO-MO approximation, MO's of H_2^+ and H_2 molecule. (**8Hrs)**

Module –V

Valence bond theory, Heitler-London theory, electron density distributions,
the Ab-initio calculations semiempirical methods. Huckel theory for linear and cyclic conjugated systems;
Applications to simple π systems: Ethylene, vinyl, cyclopropenyl. (**8Hrs)**

Text Books / Reference Books:

1. Quantum Chemistry – Levine
2. Quantum Chemistry – R K Prasad
3. Molecular Quantum Mechanics – P.W.Atkins
4. Quantum Chemistry – Pauling & Wilson
5. Quantum Chemistry – F.L.Pilar
6. Quantum Chemistry – McQuarrie
7. Quantum Chemistry – Eyring, Walter and Kimball

Chemistry of Nanomaterials
Subject Code: CH20304A (with effect from January 2023)

Credit 4 **Contact hours:** 4 hrs/week

Objectives: The course introduces the concept of nano science, specifically nano material chemistry and its applications.

Course Outcome:
CO1: Understanding of basics of nanomaterials.
CO2: Ability to generate new methods for synthesis of nanomaterials.
CO3: Knowledge of various experimental techniques and characterizations of nanomaterials.
CO4: Applications of nanomaterials in various fields of chemistry.

Module - I

Basic aspects at nanoscale materials. Surface plasmon effect, semiconductor nanoparticles, quantum confinement, magic number in clusters, physical chemistry of solid surfaces and at the nanoscale, surface (electrostatic and steric stabilization), bottom-up synthesis approach, nucleation theory, growth mechanisms and its control, Ostwald ripening, Fundamentals of film growth, nucleation process in film formation, CVD, L-B, sol-gel techniques in film deposition, micro and mesoporous materials: synthesis, formation mechanism, different applications. **(10Hrs)**

Module - II

Nanomaterial Synthesis: Chemical routes, electrochemical methods and vapor growth. Thin films methods: chemical vapor deposition, physical vapor deposition (sputtering, laser ablation) and Langmuir-Blodgett growth. Mechanical methods: ball milling and mechanical attrition. Sol-gel methods. **(7Hrs)**

Module - III

Special nanomaterials: carbon nanotubes, fullerenes, nanowires, porous silicon. Bio-inspired synthesis, Nanocomposite fabrication and Nanolithography. **(3Hrs)**

Module - IV

Overview of different experimental techniques for structural characterization of nanomaterials, Detail of the characterization techniques: X-ray diffractometry (XRD), Scherrer equation, crystal size measurement, transmission electron microscopy (TEM), bright-filed and dark field imaging in TEM, selected area electron diffraction, scanning electron microscopy (SEM), BET surface area measurement, small angle X-ray scattering, scanning tunneling microscopy (STM), atomic force microscopy (AFM), Raman spectroscopy. **(10Hrs)**

Module - V

Different applications of nanomaterials like in catalysis, environmental, biomedical, solar cells, electronic circuits, light emitting devices, data storage, biological tags, cancer treatments, drug delivery. **(10Hrs)**

Texts Books / Reference Books:

1. "Inorganic Materials Synthesis and fabrication" by John N. Lalena. John Wiley and Sons.
2. "Nanochemistry: A chemical approach to nanomaterials" by Geoffrey A. Ozin and Andre C. Arsenault. RSC Publishing.

Supramolecular Chemistry
Subject Code: CH20305A (with effect from January 2023)

Credit 4 **Contact hours:** 4 hrs/week

Objective – Introduction to concepts of Supramolecular chemistry, various routes of synthesis, its uses and future possible application.

Course Outcome:
CO1: Understanding Host-Guest Chemistry, receptors & Macrocyclic effects
CO2: Understanding of various intermolecular forces and it application in construction of supramolecules.
CO3: Understanding chemistry of formation of various supramolecular systems and their application.
CO4: Knowledge of self-assembly process in construction of supramolecules.
CO5: Understanding the role of coordination chemistry in construction of functional supramolecular materials.

Module I

Introduction: From molecular to supramolecular Chemistry, Factors leading to strong binding, H-bonding and stacking interaction, Host-Guest Chemistry, Development, Classification of Supramolecular Host-Guest Compounds, Receptors, Coordination and the Lock and Key analogy, Chelate and Macrocyclic effects. **(8Hrs)**

Module II

Nature of Supramolecular interactions: Ion-Ion, Ion-Dipole, Dipole-Dipole, Hydrogen Bonding, Cation-π Interaction, π-π Interaction, Hydrophobic effect, Van der Waals Bonding Interaction, Cooperativity, Allosteric Systems. **(8Hrs)**

Module III

Supramolecular Systems: Crown ethers, Podands, Cryptands, Spherands, Lariat ethers, Bibracchial Lariat ethers. Introduction, Synthesis, Nomenclature, Solution behaviour and application in specific recognition process. **(8Hrs)**

Module IV

Supramolecular Assembly of Complex Architectures: Novel Supramolecular Architectures – Catenanes, Rotaxanes, Knots, Cyclodextrins, Cyclophanes, Siderophores. Porphyrins and its Derivatives for construction of Supramolecular Assemblies**.** **(8Hrs)**

Module V

Coordination Chemistry Based Approach for Functional Supramolecular Materials - Weal Link Approach, Self-Assembled Molecular Flasks, Molecular Flasks as reaction vessels and containers.

(8Hrs)

Texts Books / Reference Books:

1. Supramolecular Chemistry by J.W. Steed & J.L. Atwood, published – Wiley
2. Supramolecular Chemistry by J.M. Lehn, published – Wiley – VCH
3. Review Articles

a) Development of a Coordination Chemistry- Based Approach for Functional Supramolecular Structures– Account of Chemical Research, Vol.38, No.11, 825-837, 2005
b) Multivalency and Cooperativity in Supramolecular Chemistry– Account of Chemical Research Vol.38, No.9.,723-732,2005
c) Functional Molecular Flasks: New Properties and Reactions within Discrete, Self-Assembled Hosts– Angew Chem.Int.Ed., 48, 3418-3438, 2009

Medicinal Chemistry
Subject Code: CH20306A (with effect from January 2023)

Credit 4 **Contact hours:** 4 hrs/week

Objective: This paper will introduce about drug design and their synthetic approach. Moreover, Cell structure, Protein structure, Drug action, RNA, DNA, Prodrugs etc will also be discussed. This will also give the idea of various syntheses and applications of Antipyretic Analgesics, Antibacterial agents, Antibiotics, Anti-ulcer agents, Local - Anaesthetics, Anti-cancer agents and Antimalarial.

Course Outcome:
CO1: In-depth understanding of mode of action of drugs.
CO2: Synthesis and ability to establish structure-activity relationships of various classes of drug.
CO3: Understanding the role and function of Antihistaminics.
CO4: Expertise in synthesis and classifications of various classes of local Anaesthetics.
CO5: In-depth understanding of various classes of Antimalarial drugs.

Module - I

Introduction **(10 Hrs)**
Cell structure and Protein structure. Pharmacodynamic, pharmacokinetic (drug adsorption, distribution, metabolism, and elimination) and toxicological aspects of stereoisomers (Geometrical, optical, and conformational). Drug action at Proteins, Drug action at enzymes, competitive and non-competitive inhibitors, Drug action at receptor, the drug receptor, the drug receptor interaction. Stages of drug discovery, lead discovery, identification, validation, and diversity of drug targets. Structure-activity relationships: Strategies in drug design. QSAR and combinatorial synthesis. Optimization of drug-target interactions and access to drug targets.

Antipyretic Analgesics **(3 Hrs)**
Aniline and p-Aminophenol – Paracetamol, Phenacetin, Acetanilide. Salicylic acid analogues – Aspirin, Salol. N-Aryl anthranilic acid -- Mefenamic acid, Meclofenamate sodium.

Module - II

Antibacterial Agents **(4 Hrs)**
The bacterial cell, Mechanisms of antibacterial action. Sulphonamides and Sulphones – Development of sulphonamides as drug – Protonsil, sulphapyridine. Sulphonamides for general infection – Sulphanilamide, Sulphapyridine, Sulfathiazole, Sulfadiazine. Sulphonamides for Urinary infections – Sulfacetamide. Sulphonamides for Intestinal Infections – Phthalyl sulfathiazole, Succinyl sulphathiazole. Sulphonamides for Local Infection – Sulfacetamide, Mafenide. Sulphones --- Dapsone.

Antibiotics **(3 Hrs)**
The Penicillin, General introduction to β- lactam antibiotics – Cephalosporins, Chloramphenicol, Tetracyclines – structure action relativity.

Module - III

Local Anesthetics **(6 Hrs)**
Esters – Ethyl *p*-aminobenzoate, Butamben, Procaine hydrochloride, Tetracaine hydrochloride. Piperidine or Tropone derivatives – Eucaine, Benzamine hydrochloride. Amides – Lignocaine, Prilocaine, Mepivacaine hydrochloride, Pyrrocaine hydrochloride. Miscellaneous Type – Phenacaine hydrochloride, Eugenol, Mode of action of some selected local anesthetics.

Module - IV

Antihistaminics **(6 Hrs)**
Histamine H1-receptor Antagonists – Aminoalkyl ethers, Ethylenediamines, Thiophene derivatives, Cyclic basic chain analogues. Histamine H2 Receptor blockers - Peptic ulcers, Histamine Cimetidine – a rational approach to drug design, Cimetidine, ranitidine, famotidine and nizatidine.

Module - V

Antimalerials **(8 Hrs)**
Prevention of malaria, malarial parasites, Plasmodia, and their life cycle. 4-aminoquinoline – Structure activity relationship, chloroquine, Sontoquine. 8-amonoquinolines – structure activity relationship, pamaquine, primaquine – synthesis, absorption, distribution and excretion, toxicity, uses, routes of administration and dosage. 9-Aminoacridines – Mepacrine hydrochloride, Pyrimidines – Pyrimethamine.

Texts Books / Reference Books:

1. An Introduction to Medicinal Chemistry – Graham L. Patrick (Oxford)
2. Medicinal Chemistry – Ashutosh Kar