

M.Sc. Chemistry Syllabus

Course Code	Credits	Course
CHEM-710	3	QUANTITATIVE ANALYTICAL METHODS
CHEM-711	3	INORGANIC CHEMISTRY-I
CHEM-712	3	ORGANIC CHEMISTRY-I
CHEM-713	3	PHYSICAL CHEMISTRY-I
CHEM-714	3	ANALYTICAL CHEMISTRY-I
CHEM-721	3	INORGANIC CHEMISTRY-II
CHEM-722	3	ORGANIC CHEMISTRY-II
CHEM-723	3	PHYSICAL CHEMISTRY-II
CHEM-724	3	ANALYTICAL CHEMISTRY-II
CHEM-780	1	SEMINAR - I
CHEM-811	3	INTRODUCTION TO SPECTROSCOPY
CHEM-812	3	CHROMATOGRAPHIC TECHNIQUES
CHEM-813	3	CHEMISTRY OF COORDINATION COMPOUNDS
CHEM-814	3	POINT GROUP & GROUP THEORY
CHEM-815	3	MOLECULAR REARRANGEMENT
CHEM-816	3	BIO- ORGANIC CHEMISTRY
CHEM-817	3	BIOENERGETICS
CHEM-818	3	STATISTICAL THERMODYNAMICS
CHEM-821	3	ADVANCED SPECTROSCOPY
CHEM-822	3	NANOCHEMISTRY
CHEM-823	3	ELETRONIC STRUCTURE, SPECTRA AND MAGNETIC PROPERTIES OF TRANSITION METAL COMPLEXES.
CHEM-824	3	CHEMISTRY OF LANTHANIDES & ACTINIDES
CHEM-825	3	PHOTOCHEMISTRY & ORGANIC REACTIONS
CHEM-826	3	ORGANIC POLYMERS
CHEM-827	3	QUANTUM CHEMISTRY
CHEM-828	3	MATHEMATICAL ASPECTS OF PHYSICAL SPECTROSCOPY
CHEM-880	1	SEMINAR – II
CBBI-802	3	CHEMOINFORMATICS

CHEM-710

QUANTITATIVE ANALYTICAL METHODS

Credits 3(2-0-2)

UNIT I: Introduction to Quantitative Analytical Methods.

UNIT II: Errors, Precision & Accuracy in Analytical Methods.

UNIT III: Classical methods in Analysis – Gravimetric, Volumetric – Neutralization titrations, complexometry & Iodometry.

UNIT IV: Electrochemical Methods – Redox Titration, Potentiometry, Thermogravimetry, Coulometry, Voltametry.

UNIT V: Colorimetry, Spectrophotometry.

UNIT VI: Chromatography – Adsorption, Partition, Gel filtration, Ion exchange.

Books Recommended:-

1. Analytical Chemistry by Gary Christian (Wiley)
2. Quantitative Analysis by Day and Underwood (Prentice Hall)
3. Instrumental Methods of Chemical Analysis by B. K. Sharma
4. Instrumental methods of Analysis by Willard, Merritt, Dean, Settle (CBS).

CHEM-711

INORGANIC CHEMISTRY-I

Credits 3(2-0-2)

UNIT I: Atomic & Molecular Structure and Chemical Bonding Atomic structure, orbitals, electronic configuration of atoms L-S coupling, periodic properties of elements, ionic radii, ionization potential, electron affinity, electro negativity, concept of hybridization. Molecular orbitals and electronic configuration of homonuclear & heteronuclear diatomic molecules. Shapes of polyatomic molecules, VSEPR theory, types of chemical bond.

UNIT II: Introduction to s, p, d, f-block elements General characteristics of each block, chemical principles involved, in extraction and purification of iron, copper, lead, zinc and aluminum; sandwich compounds, metal carbonyls and metal clusters. Rare gas- compounds, non- stoichiometric oxides.

UNIT III: Nuclear Chemistry Radioactive decay and equilibrium, Nuclear reactions, Q-value, cross sections, types of reactions, chemical effects of nuclear transformations, fission and fusion, fission products and fission yields. Radioactive techniques, tracer techniques, neutron activation analysis, counting techniques such as GM, ionization and proportional counter.

Practical:

1. Qualitative analysis of inorganic mixtures including rare earth elements.
2. Qualitative analysis of inorganic mixture with interfering acid radicals.

Books Recommended:

1. Inorganic Chemistry by Shriver & Atkins (Oxford)
2. Text book of inorganic Chemistry by P.L. Soni (S.Chand)
3. Advanced Inorganic Chemistry by Gurdeep Raj
4. Practical Inorganic Chemistry by Vogel (CBS)
5. University Practical Chemistry by PC Kamboj (Vishal Publication)

Chem-712

ORGANIC CHEMISTRY I

Credits 3(2-0-2)

UNIT I:Classes of organic compounds , homologous series,IUPAC nomenclature of alkanes,alkenes,cycloalkanes,alkynes,alcohols,ethers,ketones,aldehydes,carboxylic acids and their derivatives,amines, sulphonic acids, nitro compounds, organometallics and aromatic compounds.

2. Nomenclature of some compounds occurring in plants-anthocyanins, flavonols, isoflavones, quinones and heterocyclic compounds.

UNIT-II Organic Reactions And Mechanisms

1.Reactive Intermediates-Formation and stability of carbonium ion, carbanion,carbenes,nitrenes,radicals and arenes.

2.Types of reactions- Nucleophilic, electrophilic, radical substitution,addition and elimination reactions

3.Familiar Name Reactions- Diel's Alder,Skraup synthesis, Friedal Craft Reaction, Cannizaro Reaction, Reformatsky Reaction, Perkin Rearrangement, Michael addition, Knoevenagel reaction, Fries rearrangement, Claisen condensation, Dieckmann condensation, Baeyer Villiger reaction, Hofmann degradation, aldol condensation, Benzoin condensation, Wittig reaction.

UNIT-III Chirality And Stereochemistry Of Organic Compounds Recognition and elements of symmetry chiral structure,RS Nomenclature, Diastereomers in acyclic and cyclic systems, E-Z Isomerism, Conformational Analysis of simple cyclic (Chair and Boat form cyclohexanes)and acyclic systems. Interconversion of Fischer, Newman and Sawhorse Projection.Optical activity in absence of chiral C (Biphenyls, allenes, and spirans)

UNIT-IV Heterocyclic Chemistry Synthesis and reactivity of furan, thiophene,pyrrole,pyridine, quinoline,iso quinoline and indole; skraup synthesis, Fischer-indole synthesis.

Practical

1.Identification of various compounds with different functional groups
-Acids, carbohydrates, phenols, aldehyde, ketones, amides and hydrocarbons

Books Recommended

1. Organic chemistry by Morrison and Boyd
2. A logical approach to modern organic chemistry-Jagdamba Singh and Anand Vardhan
3. Advanced Organic Chemistry Reaction, Mechanism and structure – Jerry March
4. A Guidebook to mechanism in Organic Chemistry-Peter Sykes

CHEM-713

Physical Chemistry I

Credits 3(2-0-2)

UNIT I:Acids and Bases- Bronsted and Lewis acids and bases, pH and pKa, acid base concept in non aqueous media, HSAB concept, buffer solutions, concepts of indicators.

UNITII:Ideal and non ideal solutions:- Excess functions, activities, concepts of hydrogen number:, activities in electrolytic solution; Solution of liquids in liquids, Raoult's law, vapour pressures of ideal solutions, Colligative properties of dilute solutions, process of osmosis and laws of osmotic pressure.

UNIT III:Chemical Thermodynamics:- first law of thermodynamics, relation between C_p and C_v , Enthalpies of physical and chemical changes, Temperature dependence of enthalpies. Second law of

thermodynamics, Entropy, Gibbs Helmholtz equation. Third law of thermodynamics and calculation of entropy.

UNIT IV:Reaction kinetics:- Methods of determining rate laws, mechanism of photochemical reactions, Chain and oscillation reaction. Collision theory of reaction rates; Steric factor, treatment of unimolecular reaction, theory of absolute reaction rates, comparison of results with Eyring and Arrhenius equation. Ionic reaction; salt effect.

Practical:-

1. To study the kinetics of decomposition of sodium thiosulphate by mineral acids
2. To study the kinetics of dissolution of Mg in dilute HCl
3. To determine the velocity constant for the hydrolysis of Methyl acetate, catalysed by hydrogen ions.
4. Determination of concentration of unknown solution using drop weight method.
5. Determination of λ_{max} of KMnO_4 solution and findings the concentration of unknowns solutions by using absorptions photometer.
6. Determine the comparative viscosity of different liquids.
7. Determination of iron with KMnO_4
8. Determination of iron by $\text{K}_2\text{Cr}_2\text{O}_7$ (using external indicators)

Books Recommended:-

1. Bahel, Dubey, Nath
2. P.c. Kamboj
3. Pandey, Bajpai, Giri
4. Puri, Sharma, Pathania
5. Bahel and Tuli
6. Gurdeep Raj
7. K.L. Kapoor

CHEM-714

ANALYTICAL CHEMISTRY-I

Credits 3(2-0-2)

UNIT I:Introduction to Analytical Chemistry- Methods of qualitative and quantitative analysis.

UNIT II:Data Analysis: Errors, Accuracy, Precision, Distribution of Random errors, Statistical methods for finite samples, students 't' test confidence interval, testing for significance (F- test, 'z²' test), rejection of observation (Q- test), propagation of errors, significant figures, method of least square.

UNIT III:Colorimetric and Spectrophotometric Techniques:Principle, Lambert-Beer's law, Absorption law, Deviation from Beer's law, Instrumentation. Single beam and split beam instruments. Applications of Colorimetry and Spectrophotometry.

UNIT IV:Thermal Analysis: Introduction, types and applications of thermo analytical methods, Thermo gravimetric, Differential Thermal Analysis.

UNIT V:Light Scattering Techniques: Introduction, Mechanism of light scattering, Turbidimetry, Nephelometry.

Practical:-

1. Preparation of standard solutions and standardization of unknown solutions.
2. Volumetric and Gravimetric estimation of organic and inorganic compounds.
3. Verification of Beer's law and colorimetric determinations.
4. Turbiditometric determinations
5. Instrumentation of Spectrophotometer

Books Recommended:-

1. Analytical Chemistry by Gary Christian (Wiley)
2. Quantitative Analysis by Day and Underwood
3. Instrumental Methods of Chemical Analysis by B. K. Sharma
4. Instrumental methods of Analysis by Willard, Merritt, Dean, Settle (CBS).

CHEM-721

INORGANIC CHEMISTRY -II

Credit:3(2-0-2)

UNIT I: Chemistry of Non Transition Elements. General discussion on the properties on non transition elements, special features of individual elements synthesis, properties and structure of their halides and oxides, polymorphism of carbon, phosphorous and sulphur synthesis , properties structure of boranes, carboranes, borazines, silicates, carbides, silicones, phosphazene, sulphur-nitrogen compounds, compounds of boron, carbon and sulphur.

UNIT II: Chemistry of Transition Elements

(a)Stability constant of complexes and their determination, stabilization of unusual oxidation states. Jahn Teller effect, Interpretation of electronic spectra including charge transfer spectra, spectrochemical series, nephelauxetic series.

(b)Magnetism : Di, para, ferro and antiferromagnetism, quenching of orbital angular moment, spin orbit coupling, inorganic reaction mechanisms substitution reactions, trans effect and electron transfer reactions. Photochemical reaction of chromium and ruthenium.

UNIT III: Bio- Inorganic Chemistry Metal ions in biology, molecular mechanism of ion transport across membrane, inophores and photosynthesis, nitrogen fixation, oxygen uptake, proteins and cytochromes and ferredoxin.

Practical

1. Volumetric estimation using EDTA, Ammonium vanadate, ceric sulphate, chloramines-t and potassium iodate.
2. Colorimetric determination of Cr, Fe, Mn, Ni, Ti, W and Cu.
3. Preparation of metal complexes.

Books Recommended :

1. Theoretical Inorganic Chemistry by M.C. Day and J. Selbin,
2. Modern Aspects of Inorganic Chemistry by H.J. Emelens and A.G. Sharp.. (Van).
3. Text book of Inorganic Chemistry by P.L. Soni (S. Chand)
4. Inorganic Chemistry by Shriver & Atkins
5. Text book Quantitative Inorganic Analysis by A.I. Vogel
6. Experimental Inorganic Chemistry by W.G. Parmer

CHEM-722**ORGANIC CHEMISTRY-II****Credits 3(2-0-2)**

UNIT-I : Pericyclic Reactions Selection rules, stereochemistry of electrocyclic reaction, cycloaddition and sigmatropic shifts, Sommelet, Hauser, cope and claisen rearrangement.

UNIT-II : Alkaloids And Terpenoids Familiarity with methods of structure elucidation and biosynthesis of alkaloids and terpenoids

UNIT-III : Polyphenols Classification, Properties and uses

UNIT-IV : Introduction Of Bioorganic Molecules Elementary structure and function of carbohydrates, proteins and nucleic acid

PRACTICAL

1. Separation of mixtures containing two compounds
2. With (a) water (b) NaHCO_3 (c) NaOH
3. Determination of Saponification and Iodine value of oil sample.
4. Qualitative method for the identification of aqueous solutions of carbohydrates- Glucose, fructose, starch, sucrose, lactose and maltose

Books Recommended:

- (1) Organic Chemistry by J.L. Finar
- (2) Organic Chemistry by O.P. Agarwal

CHEM- 723**PHYSICAL CHEMISTRY II****Credits 3(2-0-2)**

UNIT- I: Advanced Electrochemistry Electrochemical cells reactions, Nernst eq. Electrode kinetics, electrical double layer, electrode electrolyte interface, batteries, primary and secondary fuel cells, types of reversible electrodes, corrosion and corrosion preventions.

UNIT-II: Physical chemistry of polymers and macro molecules number- average and weight average molecular weight, determination of molecular weight, kinetics of polymerization and its mechanism.

UNIT-III: Thermo Chemistry Heat of reaction, heat of Combustion, heat of Solution, heat of Neutralization, energy change during transition or phase change, heat of fusion, heat of Vaporization, heat of Sublimation, heat of Transition, Hess's law of heat Summation and its applications.

UNIT-IV: Colloidal Chemistry Characteristics of lyophilic and lyophobic solution, preparation, purification and properties (optical, kinetics and electrical), Gold number, electrophoresis, associated colloid, cleaning action of soap and detergents, emulsion, gels and its application.

Practical:

1. The rate constant of reaction between acetone and iodine in presence of mineral acid and a catalyst and to show that this reaction with respect to iodine is of zero order.
2. The absorption of aqueous acetic acid by activated charcoal and to study the absorption isotherm.
3. To prepare the solution of Arhenius sulphide, ferric hydroxide, Sulphur and Aluminum hydroxide solution.
4. To determine the heat of Neutralization of NaOH and HCl.
5. To determine the molecular weight of the given substance (Glucose/Sucrose/Urea etc). cryscopically using water as the solvent with the help of Beckmann's thermometer.
6. Determination of rate constant of the hydrolysis of methyl acetate by Sodium Hydroxide.

Books Recommended:-

1. Puri, Sharma, Pathania
2. Bahl and Tuli
3. Gurdeep Raj
4. K.L. Kapoor

CHEM-724

ANALYTICAL CHEMISTRY II

Credits 3(2-0-2)

UNIT I :Introduction to Separation Techniques: Solvent extraction, ion exchange methods, Chromatography (paper, TLC, Column)

UNIT II : Electro Analytical Techniques: Voltametry, Polarography, Amperometry, Coulometry, Conductometry, Potentiometry.

UNIT III : Diffraction Techniques: Introduction, types and application

UNIT IV : Electrochemical Techniques:Introduction and application of Electrolysis, Electrophoresis

Practical:-

1. Separation of ions and molecules by solvent extractions
2. Preparation of solvent systems and T.L.C. plates
3. Separation of amino acids, sugars and ions by paper chromatography.

Books Recommended:-

1. Analytical Chemistry by Gary Christian (Wiley)
2. Quantitative Analysis by Day and Underwood
3. Instrumental Methods of Chemical Analysis by B. K. Sharma
4. Instrumental methods of Analysis by Willard, Merritt, Dean, Settle (CBS).

CHEM-811

INTRODUCTION TO SPECTROSCOPY

Credits 3(3-0-0)

UNIT I : Electromagnetic Radiations:- Interaction of EM-radiations with matter, scattering, dispersion and transmission of radiation.

UNIT II : UV-Visible Spectroscopy:-Nature of electronic excitation, origin of UV- band structure, principle of adsorption spectroscopy, instrumentation, presentation of spectra chromophore, Woodward Fieser rules for dienes.

UNIT III : IR (vibrational) Spectroscopy:- Infra red absorption process, stretching and bending, Infra Red Spectrometer, IR-Spectrum, application of IR Spectrum.

UNIT IV : Mass Spectrometry:- Basic principles, theory, instrumentation, mass spectrum, the nitrogen rule, general fragmentation modes, important features in mass spectroscopy, simple problems in mass spectroscopy.

UNIT V : Application of UV –Visible, IR and Mass Spectroscopic techniques for structure elucidation of compounds.

Books Recommended:-

1. Spectroscopy- Pavia, Lampman, Kriz, Vyuyan.
2. Elementry Organic Spectroscopy by Y.R. Sharma
3. Spectroscopy by P.S. Kalsi
4. Spectroscopy by H.Kaur.
5. Organic Spectroscopy by William Kemp
6. Spectroscopic Methods by Sylverstein.

CHEM-812 CHROMATOGRAPHIC TECHNIQUES Credits 3(2-0-2)

UNIT I : Partition Chromatography: Paper chromatography, Thin Layer Chromatography, Rf value, chromatogram, single, 2D and 3D chromatography. Ascending and descending chromatography. Applications of partition chromatography.

UNIT II : Adsorption Chromatography:- Principle, classification of column chromatography, column efficiency, preparation of column.

UNIT III : On Exchange Chromatography:- Structure of ion exchanger, types of cation and anion exchanger, mechanism of ion exchange chromatography. Ion exchange resins, ion exchange capacity. Factors affecting separations, applications of IEC.

UNIT IV : Exclusion Or Gel Chromatography:- Technique in Gel Chromatography, Gel preparation, packing of column, theory and application of gel chromatography

UNIT V : H.P.L.C.:- Principle, instrumentation, advantages of HPLC, Effect of temperature in HPLC, HPTLC, Applications of HPLC and HPTLC.

UNIT VI : Gas Chromatography:- Principle, G.C. columns, Instrumentation, Methodology, GC-MS, applications of GC.

Practical:- 1. Separation of Ions, molecules by descending (2D, 3D) Chromatography.

1. Separation of molecules by Column Chromatography.
2. Separation of ions using ion exchangers

Books Recommended:-

1. Analytical Chemistry by Gary Christian (Wiley)
2. Quantitative Analysis by Day and Underwood
3. Instrumental Methods of Chemical Analysis by B. K. Sharma
4. Instrumental methods of Analysis by Willard, Merritt, Dean, Settle (CBS).

CHEM-813 CHEMISTRY OF COORDINATION COMPOUNDS Credits-3(3-0-0)

Unit I: Chemistry of Coordination Compounds: Structural aspects, isomerism, crystal field splitting of d-orbital's, CFSE, magnetism and color of transition metal ions, ligand field theory.

Unit II: Organometallic Compounds: Synthesis, structure and bonding in polynuclear carbonyls with and without bridging complexes with linear π donor, ligands, complexes with cyclic π donors. Catalysis by Organometallic compounds.

Unit III: Advanced Theory of Solids: Dislocation in solids, Schottky & Frenkel's Defect, electrical properties, insulators & semiconductors, superconductors, Band theory of solids, solids state reactions.

Books Recommended :

1. Theoretical Inorganic Chemistry by M.C. Day and J. Selbin,
2. Modern Aspects of Inorganic Chemistry by H.J. Emeleus and A.G. Sharp.. (Van).
3. Text book of Inorganic Chemistry by P.L. Soni. (S. Chand).
4. Inorganic Chemistry by Shriver & Atkins (Oxford)

CHEM- 814 POINT GROUP AND GROUP THEORY

Credit:3(3-0-0)

UNIT I : Properties of a group. Point groups, Sub groups, similarity transformation, classes of symmetry transformation, similarity transformation, classes of symmetry operation, representation of group reducible and irreducible representation of group, orthogonality theorem, rules of irreducible representation and their properties.

Books Recommended:

1. Chemical Applications of Group Theory by F.A. Cotton (Inter Science).
2. Theoretical Inorganic Chemistry by M.C. Day and J. Selbin (Affiliated East, West Press).
3. Group Theory in Chemistry by V. Ramakrishna & M. S. Gopi Nathan,
4. A text book quantitative inorganic analysis by A.I. Vogel (CBS).
5. Technical Methods of Ore Analysis by A.I. Weining

CHEM-815

MOLECULAR REARRANGEMENT

Credit:3(3-0-0)

UNIT-I Selective Organic Name Reactions Hydroboration, Oppenauer oxidation, Clemmensen reduction, Wolf-Kishner reaction, Meerwein-Ponndorf-Verley, Birch reduction, Favorskii reaction, Stark enamine reaction, Mannich reaction, Sharpless asymmetric epoxidation, Ene reaction, Barton reaction, Hofmann-Löffler-Freytag reaction, Shapiro reaction, Chichibabin reaction.

UNIT-II Reagents In Organic Synthesis

1. Complex metal hydrides
2. Osmium tetroxide
3. Selenium dioxide
4. Grignard reagent
5. Lithium Aluminium Hydride
6. Anhydrous aluminium chloride

Books Recommended:

1. Organic Reactions & their mechanism by P.S. Kalsi
2. Organic reaction Vol I by Aditi Sangal
3. Reaction & Reagents by O.P. Agarwal

CHEM-816

BIO-ORGANIC CHEMISTRY

Credit:3(2-0-2)

UNIT-I Vitamins Coenzymes-their chemistry and activity in biological systems.

UNIT-II Steroids And Hormones Chemistry and Biological activity of steroids and hormones. Plant and animal hormones.

UNIT-III Pigment And Dyes Chemistry, classification and application of dyes and pigments

UNIT-IV Drugs Classification, brief Chemistry and application of important drugs

Practical

1. Separation of amino acids by Thin layer chromatography method
2. Synthetic preparation and yield determination of
 - (a) Benzamide from benzoyl chloride
 - (b) Picric acid from phenol
 - (c) Osazone derivative from glucose
 - (d) Benzoate derivative of phenol
 - (e) Preparation of dye from nitrobenzene
3. Extraction of essential oil by Cleavanger's apparatus.

Books Recommended:

- (1) Fundamental concepts of Applied Chemistry by Jayashree Ghosh

CHEM.-817

BIOENERGETICS

Credit:3(3-0-0)

UNIT I : Concept of energy, Thermodynamic principles, free energy changes and equilibrium constants, standard free energy values and chemical reaction, coupled reaction, electron transport carriers, interconnections of energy, role of electron transport energy.

Books Recommended:-

1. Biochemistry by J. L. Jain (S. Chand Publication)
2. Outlines of Biochemistry by Lehninger(Kalyani publisher)

CHEM-818

STATISTICAL THERMODYNAMICS

Credits 3(3-0-0)

UNIT I : Thermodynamics probability and entropy, Maxwell- Boltzmann, Bose- Einstein and Fermi-dirac statistics. Partition function; rotational translational, vibrational and electronic partition function for diatomic molecules; calculations of thermodynamic function and equilibrium constants. Theories of specific heat for solids.

Books Recommended:-

1. Physical chemistry Vol 5 by K.L.Kapur
2. Elements of Physical Chemistry by Puri Sharma Pathania

CHEM-821

ADVANCED SPECTROSCOPY

Credits 3(3-0-0)

UNIT I Introduction and Principles: The failures of classical physics, Wave – particle duality, Impact on biology: Electron microscopy, Information in a wave function, Uncertainty Principle, The Postulates of quantum mechanics.

UNIT II Translational Vibrational & Rotational Motions: A particle in a box, motion in two or more directions, tunneling, The energy levels, The wave functions, Rotations in two dimensions a particle on a ring, Rotation in three dimensions: the particle on a sphere, Impact on nano science.

UNIT III Techniques of approximation: The structure of hydrogenic atoms, atomic orbitals and their energies, spectroscopy transitions and selection rules, The orbital approximation, self-consistent field orbitals.

Books Recommended

1. Physical Chemistry by Atkins
2. Elements of Physical Chemistry by Puri Sharma, Pathania
3. Essentials of Physical Chemistry by Babl and Tulli

CHEM-828 MATHEMATICAL ASPECT OF SPECTROSCOPY. Credits 3(3-0-0)

UNIT I : Electromagnetic radiation, atomic spectra, Molecular spectra, Absorption spectrum, Emission spectrum, various types of spectra, Basic features of spectrometers, Rotational or microwave spectra, Vibrational spectra, Rotation – vibration spectra.

UNIT II: IR spectrometer, IR spectroscopy applications of- Raman Scattering: Raman effect, Raman spectra, Raman spectroscopy-experimental.

UNIT III: Electronic spectra, Absorption of light and colour of compounds, Colour of compounds dependence on electronic transition, colour of organic compounds. Batho chromic effect, Hypso chromic effect, Auxochromic effect, Vibrational structure of electronic spectra, Electronic spectra of chromophores: Treatment based on MO Theory.

UNIT IV: NMR spectroscopy- experimental technique, chemical shifts, shielding and deshielding of protons, Nuclear spin spin interaction, fourier- transform (FT) NMR spectroscopy, Electron spin resonance (ESR) spectroscopy, Hyperfine structure in ESR spectra, Mossbauer spectroscopy, photoelectron spectroscopy (PES).

Books Recommended

1. Physical Chemistry by Atkins
2. Elements of Physical Chemistry by Puri Sharma, Pathania

CBBI-802

Chemoinformatics

Credits 3(2-0-2)

UNIT I : Role of computers in chemical research, Introduction to Chemoinformatics, Representation and manipulation of 2D and 3D molecular structures, Chemical Databases- Design, Storage & Retrieval methods.

UNIT II : Reaction databases, Representation of chemical reactions, Search techniques(Full, Sub and Super structure), Similarity searches, Modeling of small molecules.

UNIT III : Combinatorial chemistry and Library design –Introduction, Data visualization, Data mining methods, Prediction of ADMET properties, Chemoinformatics tools for drug discovery.

Practical:

1. To draw and analyze the chemical structures by using the ChemSketch/ChemDraw software.

2. To convert the chemical structure data from one file format to other file formats by using the CHIMERA/BABEL software.
3. To study about the different types of chemical structure database.
4. To visualize the chemical structure in different views by using the visualization softwares.
5. To calculate the descriptors of few ligands by using the DRAGON software.
6. To perform the virtual screening of ligands by using the AUTODOCK programme.

Books Recommended

1. An Introduction to Chemoinformatics by Andrew R. Leach, V.J. Gillet
2. Chemoinformatics by Johann Gas teiger
3. Chemoinformatics: Theory, Practice & Products by Bunin., Siesel, B., Morales, G., Bajorath, J.