

Course outcomes:

After completion of the course, the learner shall be able to understand:

C01: Important mathematical concept widely applied in chemistry

C02: numerical methods for differentiation and integration

C03: Computer Programming

C04: Curve fitting methods

C05: Different software used in data handling and analysis **Course Content:**

Unit 1**[12 Lectures]**

Mathematics:

Fundamentals, mathematical functions, polynomial expressions, logarithms, the exponential function, units of a measurement, interconversion of units, constants and variables, equation of a straight line, plotting graphs.

Uncertainty in experimental techniques: Displaying uncertainties, measurements in chemistry, decimal places, significant figures, combining quantities.

Uncertainty in measurement: types of uncertainties, combining uncertainties, statistical treatment, mean, standard deviation, relative error, data reduction and the propagation of errors, graphical and numerical data reduction, numerical curve fitting: the method of least squares (regression).

Algebraic operations on real scalar variables (e.g. manipulation of van der Waals equation in different forms), roots of quadratic equations analytically and iteratively (e.g. pH of a weak acid), numerical methods of finding roots (Newton-Raphson, binary – bisection, e.g. pH of a weak acid not ignoring the ionization of water, volume of a van der Waals gas, equilibrium constant expressions).

Differential calculus: The tangent line and the derivative of a function, numerical differentiation (e.g., change in pressure for small change in volume of a van der Waals gas, potentiometric titrations).

Numerical integration (Trapezoidal and Simpson's rule, e.g. entropy/enthalpy change from heat capacity data).

Unit 2

Computer programming:

[8 Lectures]

Constants, variables, bits, bytes, binary and ASCII formats, arithmetic expressions, hierarchy of operations, inbuilt functions, elements of the BASIC language, BASIC keywords and commands, Logical and relative operators, strings and graphics, compiled versus interpreted languages, Debugging, simple programs using these concepts, matrix addition and multiplication, statistical analysis.

BASIC programs for curve fitting, numerical differentiation and integration (Trapezoidal rule, Simpson's rule), finding roots (quadratic formula, iterative, Newton-Raphson method).

Unit 3

[4 Lectures]

HANDS ON:

Introductory writing activities: introduction to word processor and structure drawing (ChemSketch) software, incorporating chemical structures, chemical equations, and expressions from chemistry (e.g. Maxwell-Boltzmann distribution law, Bragg's law, van der Waals equation, etc.) into word processing documents.

Unit 4

HANDS ON:

[4 Lectures]

Handling numeric data:

Spreadsheet software (Excel), creating a spreadsheet, entering and formatting information, basic functions and formulae, creating charts, tables and graphs, incorporating tables and graphs into word processing documents, simple calculations, plotting graphs using a spreadsheet (Planck's distribution law, radial distribution curves for hydrogenic orbitals, gas kinetic theory- Maxwell-Boltzmann distribution curves as function of temperature and molecular weight), spectral data, pressure-volume curves of van der Waals gas (van der Waals isotherms), data from phase equilibria studies, graphical solution of equations.

Unit 5

[4 Lectures]

HANDS ON:

Numeric modelling:

Simulation of pH metric titration curves, Excel functions LINEST and Least Squares, Numerical curve fitting, linear regression (rate constants from concentration time data, molar extinction coefficients from absorbance data), numerical differentiation (e.g. handling data from potentiometric and pH metric titrations, pKa of weak acid), integration (e.g. entropy/enthalpy change from heat capacity data).

Unit 6

[4 Lectures]

Statistical analysis:

Gaussian distribution and errors in measurements and their effect on data sets.

Descriptive statistics using Excel. Statistical significance testing: The *t* test, the *F* test.

Text Book(s)

1. McQuarrie, D. A. *Mathematics for Physical Chemistry*, (University Science Books, 2008).
2. Harris, D. C. *Quantitative Chemical Analysis*. 7th Edn., (Freeman, 2010).
3. Levie, R. de, *How to use Excel in analytical chemistry and in general scientific data analysis*, (Cambridge University Press, 2001).
4. Venit, S.M. *Programming in BASIC: Problem solving with structure and style*, 2nd Edn. (Jaico Publishing House, 2001).

Reference Book(s)

1. Mortimer, R. *Mathematics for Physical Chemistry*, 4th Edn., (Elsevier, 2013).
2. Steiner, E. *The Chemical Maths Book* (Oxford University Press, 2008).
3. Yates, P. *Chemical calculations*, 2nd Edn., (CRC Press, 2007).

Unit 1

Separation techniques of organic compounds and their spectroscopic identification. Experiments involving the separation and purification of organic compounds from a mixture, using chromatographic techniques, steam distillation, fractional crystallization and sublimation.

Unit 2

Synthesis of organic compounds using common reagents: At least eight preparation (involving two or more than two steps) involving the following representative reactions: (a) Oxidation of alcohol, (b) Reduction of carbonyl group, (c) Nucleophilic substitution, (d) Cycloaddition reaction, (e) Condensation reaction, (f) Aromatic electrophilic substitution, (g) Preparation of dyes, (h) Heterocyclic synthesis, (i) Solid phase synthesis etc.

Unit 3

Natural product extraction: Caffeine, Nicotine, Carotenoids etc.

Unit 4

Estimation of Glucose, acetic acid in vinegar, -OH groups etc.

Unit 5

Determination of acid value and saponification value of fat/oil.

Unit 6

Green experiments **Text**

Book(s)

1. Pasto, D., Johnson, Miller, M. *Experiments and Techniques in Organic Chemistry*, (Prentice Hall, 1992).
2. Williamson, K. L. *Macroscopic and Microscale Organic Experiments*, (D. C. Heath & Company, 1999).

Reference Book(s)

1. Furniss, B. S., Ford, A. J. H., Smith, P. W. H., Tatchell, A. R. *Vogel's Textbook of Practical Organic Chemistry*, 5th Edn., (Wiley, 1989).

Unit 1

Quantitative estimation involving volumetric (redox and complexometry), gravimetric and spectrophotometric methods of analysis of constituents in three component mixtures, alloys and minerals.

Unit 2

Synthesis and characterization of inorganic compounds, including those involving green synthetic methodology: Characterization includes elemental analysis, studies by IR, electronic spectra, magnetic susceptibility, conductance measurements, cyclic voltammetry. TG, DSC.

Text Book(s)

1. Mendham, J., Denney, R. C., Barnes, J. D., Thomas, M. and Sivasankar, B. *Vogel's Quantitative Chemical Analysis*, 6th Edn., (Pearson Education, 2009).
2. Marr, G., Rockett, B. W. *Practical Inorganic Chemistry*, (Van Nostrand, 1972).

Reference Book(s)

1. Wollins, J. D. *Inorganic Experiments*, 3rd Edn., (VCH, 1994).
2. Parshall, G. W. (Ed. in Chief). *Inorganic Synthesis, Vol. 15*, (McGraw Hill, 1974).

On completion of this course the students will be able to understand:

C01: Instrumentation technique of various analytical tools like XRD, AAS, cyclic voltammetry, chromatography, optical and electronic microscopy

C02: Basic principles of those instrumentation techniques

C03: Application of analytical tools (XRD, SEM, TEM, TGA, AAS, ICP-OES) in characterization and elemental detection of chemical compounds: solids (crystalline, amorphous, nanomaterials), liquids and gases.

C04: Application of radiochemical techniques in chemical reactions

C05: Electrochemical techniques for understanding electron transfer reaction mechanism, fuel cell application, Li-ion battery

Course Content:**Unit 1****[4 Lectures]**

X-ray methods: X-ray diffraction, X-ray fluorescence and X-ray absorption and X-ray emission spectroscopy.

Unit 2**[4 Lectures]**

Thermoanalytical methods: Thermo gravimetric analysis, differential thermal analysis and differential scanning calorimetry.

Unit 3**[6 Lectures]**

Electrochemical methods: Coulometry, Polarography, anode-stripping voltammetry, pulse techniques, cyclic voltammetry, electrogravimetry, spectroelectrochemistry.

Unit 4**[5 Lectures]**

Chromatographic methods: Adsorption, liquid-liquid partition, ion-exchange, paper and thin-layer chromatography, HPLC, gel permeation chromatography and gas chromatography, HPTLC, Flash chromatography.

Unit 5**[4 Lectures]**

Radiochemical methods: Tracers in chemical analysis, isotopic exchange, isotopic dilution technique, labeling experiments in studying reaction mechanism.

Unit 6**[8 Lectures]**

Optical microscopy: Optical Rotatory Dispersion and Circular Dichroism: Definition, Deduction of absolute configuration, octane rule for ketones.

Transmission electron microscopy (TEM) and Scanning electron microscopy (SEM).

Unit 7**[5 Lectures]**

Atomic absorption spectroscopy: Inductively coupled Plasma- mass spectroscopy (ICPMS), ICP-AES (Atomic Emission Spectroscopy).

Text Book(s)

1. Drago, R. S. *Physical Methods in Chemistry*, (Saunders College, 1992).
2. Hollas, J. M. *Modern Spectroscopy*, (John Wiley, 1996).

Reference Book(s)

1. Willard, H. H. *Instrumental Methods of Analysis*, (East West Press, 1998).
2. Bard, A. J., Faulkner, L. R. *Electrochemical Methods, Fundamentals and Applications*, (John Wiley, 2000).

Unit 1

Purification of chemicals and calibration of analytical instruments; Error analysis- primary and secondary data, accuracy and precision, averaging of data, types of experimental error, significant figures, estimation and representation of error, and minimization of errors, Handling of basic instruments, e.g., potentiometer, conductivity meter, spectrophotometer, etc., through three basic experiments.

Unit 2

Four minor experiments chosen from: Kinetics by spectrophotometry, polarimetry and conductometry, Relative strength of two acids by conductance, Interfacial tension between two liquids by Tensiometer, Determination of a weak acid and a strong acid in mixture by potentiometry, Study of liquid-liquid phase diagram, Determination of fluoride by ion selective electrode, nitrate spectrophotometry, Determination of average molecular weight of a polymer by viscometry, etc.

Unit 3

Four major experiments chosen from: Study of non-Newtonian polymer solutions by Brookfield viscometer, Study of excess adiabatic compressibility of binary system by ultrasonic interferometry, Simultaneous determination of CMC and partition equilibrium constant by spectroscopic method, Kinetics of the catalytic decomposition of H_2O_2 by manganese (IV) oxide, Determination of CMC by Du Nouy Tensiometry, Micellar catalysis by spectroscopy, Determination of pK_a by spectroscopy, Determination of stoichiometry and the stability constant of the complex formation, Study of pseudo-ternary phase diagram of oil-water-(surfactant-cosurfactant) system, Determination of activation energy of reaction by polarometry, Preparation and characterization of nanoparticles etc.

Text Book(s)

1. Viswanathan, B., Raghavan, P. S. *Practical Physical Chemistry*, (Viva Books Pvt. Ltd., 2005).
2. James, A. M., Prichard, F. E. *Practical Physical Chemistry*, 3rd Edn., (Longman, 1974).

Reference Book(s)

1. Jadav, J. B. *Advanced Practical Physical Chemistry*, (Krishna Prakashan, 2015).
2. Garland, G. W., Nibler, J. W., Shoemaker, D. P. *Experiments in Physical Chemistry*, 7th Edn., (McGraw- Hill, 2008).

CH 516: COMPUTATIONAL CHEMISTRY AND NUMERICAL ANALYSIS L3 TO P0 CR 3

Course outcomes:

On completion of this course, the students will be able to understand:

CO1: The numerical methods of integration and differentiations

CO2: Molecular mechanics calculation of complex system

CO3: Quantum mechanical calculation of complex systems

Course Content:

Unit 1

[8 Lectures]

Data analysis, mean and standard deviation, absolute and relative errors, linear regression, covariance and correlation coefficient. Curve fitting, solution of polynomial equation, numerical integration (Trapezoidal Rule, Simpson's Rule, Gaussian Quadrature), solution of ordinary differential equations (Euler's Method, Runge-Kutta methods, predictor-corrector method), matrix multiplication, inversion and diagonalization.

Unit 2

[6 Lectures]

Molecular Mechanics: Basic geometrical description of molecules; force-field development, intermolecular interactions, origin and modelling of dispersion forces & hydrogen bonds, strengths, weaknesses and applicability of currently available forcefields.

Unit 3

[8 Lectures]

Static properties of complex systems: Introduction to Monte Carlo as a way of averaging. Metropolis Monte Carlo algorithm: introduction and applications.

Dynamical properties of complex systems: Molecular Dynamics as a way of averaging. Integration of the Newton's equations: initial conditions, numerical algorithms (Verlet and leap-frog), and thermostats.

Unit 4

[6 Lectures]

Quantum Chemistry: Many electron systems, Hartree-Fock method, basis sets, electron correlation and its treatment, basics of density functional theory, DFT based reactivity descriptors. Introduction to popular softwares (like Gaussian, DMol, GAMESS).

Applications to simple molecular systems.

Unit 5

[8 Lectures]

Combined QM/MM methods: Implications of the choice of QM and MM methods; Application of QM/MM methods in organic, inorganic and organometallic systems including bio-organic and bio-inorganic molecules.

Quantitative structure activity relation (QSAR): Early approaches, topological indices, fragmental models; quantum mechanical descriptors.

Text Book(s)

1. Lewars, E. *Computational Chemistry*, (Springer, 2003).
2. Balagurusamy, E. *Numerical Methods*, (Tata McGraw-Hill Publishing Company Limited, 2002).

Reference Book(s)

1. Leach, A. R. *Molecular Modeling: Principles and Applications*, 2nd Edn., (Pearson Prentice Hall, 2001).
2. Cramer, C. J. *Essentials of Computational Chemistry* (Wiley 2002).
3. Jensen, F. *Introduction to Computational Chemistry* (Wiley 1999).

Course outcomes:

On completion of this course, the students will be able to learn:

CO1: Environmental impact and quality parameters of air, water and soil

CO2: Analysis and purification of water, wastewater, solid-wastes and air pollution.

CO3: Environmental protection and pollution prevention

CO4: Green chemistry principles and Design of green synthesis

Course Content:

Unit 1

[6 Lectures]

Environment and chemistry; Matter and cycles of matter; The atmosphere and atmospheric chemistry: The geosphere and geochemistry; Aquatic chemistry, CO₂ distribution, acid-base and redox equilibrium in water, pE-pH curves, water quality parameters.

Unit 2

[6 Lectures]

Chemistry and environmental pollution: Chemical hazards, chemical disasters, Water pollution, air pollution and soil pollution; Industrial pollution, vehicular pollutions, agricultural pollution, pollution by plastics; environmental biochemistry, toxicological chemistry.

Unit 3

[6 Lectures]

Environmental analysis: Analysis of water and wastewater, solid-wastes and air pollution.

Unit 4

[6 Lectures]

Environmental protection: pollution prevention, green chemistry, biodegradation, water and wastewater purification – removal of arsenic, iron, fluoride, etc.; air purification, waste minimization, industrial and municipal waste treatment and soil remediation.

Unit 5

[6 Lectures]

Green chemistry principles: Principles of green chemistry, atom economy, less hazardous chemical syntheses, designing safer chemicals, safer solvents and auxiliaries, design for

energy efficiency, renewable feedstock, catalysis, design for degradation, real time analysis for pollution prevention, and inherently safer chemistry for accident prevention.

Unit 6

[6 Lectures]

Design of green synthesis: Ideal synthesis, clean routes, supercritical solvents, ionic liquids, green catalyst, auto-exhaust catalyst and clean technology Real world examples.

Text Book(s)

1. Manahan, S. E. *Environmental Chemistry*, 9th Edn. (CRC Press, Boca Raton, 2010).
2. Anastas, P. T. and Warner, J. C. *Green Chemistry: Theory and Practice*, (Oxford University Press, 1998).

Reference Book(s)

1. Hutzinger, O. *Handbook of Environmental Chemistry*, (Springer-Verlag, 1991).
2. Cann M. C., Connelly, M. E., *Real World Cases in Green Chemistry*, (ACS, 2000).

Course outcomes:

On completion of this course, the students will be able to learn:

CO1: Fundamentals of industrial polymers

CO2: Synthesis, processing and properties of some industrially important polymers CO3: Discussion of the applications of the polymeric products

Course Content:**Unit I****[4 Lectures]**

Fundamentals of industrial polymers including monomer, initiator, catalyst; manufacturing techniques, structure and property, modification, applications, etc.

Unit II**[8 Lectures]**

Industrial commodity thermoplastics like polyethylene, polypropylene, polystyrene, poly(vinyl chloride), high impact polystyrene, etc.; their preparative methods, microstructures, physical, mechanical, thermal, chemical and aging properties; various commodity to advanced applications.

Unit III**[8 Lectures]**

Industrial engineering thermoplastics like poly(acrylonitrile), nylon 6, nylon 6,6, polyesters, polycarbonates, polyurethanes, poly(tetrafluoroethylene), etc. their preparative methods, microstructures, physical, mechanical, thermal, chemical and aging properties; various commodities to advanced applications.

Unit IV**[8 Lectures]**

Industrial thermosetting resins like phenolic resins, amino-resins, alkyds, unsaturated polyesters, polyurethanes, epoxy resins, etc.; their preparative methods, microstructures, physical, mechanical, thermal, chemical and aging properties; various commodity to advanced applications.

Unit V**[8 Lectures]**

Industrial elastomers like natural rubber, styrene-butadiene rubber, acrylonitrile-butadiene rubber, synthetic isoprene rubber, isobutylene-isoprene rubber, chloroprene rubber,

ethylenepropylene diene rubber, chlorosulphonated polyethylene rubber, silicone rubber, fluororubbers, etc. their preparative methods, microstructures, physical, mechanical, thermal, chemical and aging properties; various commodity to advanced applications.

Text Books

1. P. Ghosh, Polymer Science and Technology: Plastics, Rubbers, Blends and Composites, Third Edition, McGraw Hill Education Private Limited (India), 2011
2. J. A. Brydson, Plastics Materials, 4th edn., Butterworths, London, 1982
3. J. A. Brydson, Rubbery materials and their compounds, Elsevier Applied Science, London, 1988

Reference Book

1. M. Chanda, S. K. Roy, Industrial Polymers, Specialty Polymers, and Their Applications, 1st Edition, CRC Press, 2019.
2. E. Alfredo Campo, Industrial Polymers, Carl Hanser Verlag GmbH & Co. KG, Berlin, 2007

Course Content:**Section A: Inorganic Chemistry**

1. Estimation of sodium carbonate and sodium hydrogen carbonate present in a mixture
2. Estimation of oxalic acid by titrating with KMnO_4
3. Estimation of water of crystallization in Mohr's salt by titrating with KMnO_4
4. Estimation of Fe (II) ions by titrating with $\text{K}_2\text{Cr}_2\text{O}_7$ using internal indicator
5. Estimation of Cu (II) ions iodometrically using $\text{Na}_2\text{S}_2\text{O}_3$

Section B: Organic Chemistry

1. Detection of extra elements (N, S, Cl, Br, I) in organic compounds (containing upto two extra elements)
2. Separation of mixtures by Chromatography: Measure the R_f value in each case (combination of two compounds to be given)
 - (a) Identify and separate the components of a given mixture of α -amino acids (glycine, aspartic acid, glutamic acid, tyrosine or any other amino acid) by paper chromatography
 - (b) Identify and separate the sugars present in the given mixture by paper chromatography.

Text Book(s)

1. Svehla, G., Sivasankar, B. *Vogel's Qualitative Inorganic Analysis*, 7th Edn., (Pearson Education, 2012).
2. Mendham, J., Denney, R. C., Barnes, J. D., Thomas, M., Sivasankar, B. *Vogel's Quantitative Chemical Analysis*, 6th Edn., (Pearson Education, 2009).
3. Vogel, A.I., Tatchell, A.R., Furnis, B.S., Hannaford, A. J., Smith, P. W. G., *Textbook of Practical Organic Chemistry*, 5th Edn., (Prentice-Hall, 1996).
4. Mann, F.G., Saunders, B.C. *Practical Organic Chemistry*, (Orient-Longman, 1960).

Course Content:

1. Qualitative Analysis of Inorganic Mixtures (excluding interfering radicals)
2. Preparation of Mohrs salt
3. Estimation of Glucose
4. Nitration of organic compounds
5. Reduction of functional groups
3. Preparation of buffer solution and measurement of pH
4. Viscosity measurement of solution
5. Conductometric acid-base titration
6. Measurement surface tension of liquid by stalagmometer
7. Verification of Beer-Lamberts law
8. Titration of a mixture of AcOH, HCl and CuSO₄ by conductometric method

Text Book(s)

1. Furniss, B. S., Ford, A. J. H., Smith, P. W. H., Tatchell, A. R. *Vogel's Textbook of Practical Organic Chemistry*, 5th Edn., (Wiley, 1989).
2. Jadav, J. B. *Advanced Practical Physical Chemistry*, (Krishna Prakashan, 2015).
3. Mendham, J., Danney, R. C., Barnes, J. D., Thomas, M. *Vogel's Textbook of Quantitative Chemical Analysis*, 6th Edn., (Prentice Hall, 2009).
4. Gurdeep, R. *Advanced Practical Inorganic Chemistry*, (Krishna Prakashan, 2013).

CI 209

Chemistry Laboratory-III

L O T O P 3 CR 3 Course

Content:

Unit 1

Inorganic: Qualitative Analysis of Inorganic Mixtures (including interfering radical) **Unit**

2

Physical:

1. Thermochemistry experiment (determination of heat of hydration)
2. Electrochemistry (determination of redox potential)
3. Chemical kinetics (determination of rate constant of hydrolysis of methyl acetate catalysed by an acid)
4. Conductometric/potentiometric (determination of equivalence conductance of an electrolyte at infinite dilution)
5. UV-VIS spectrophotometric (determination of dissociation constant of ferrithiocyanate complex).

Text Book(s)

1. Svehla, G. *Vogel's Qualitative Inorganic Analysis*, 7th Edn., (Prentice Hall, 1996).
2. Yadav, J. B. *Advance Practical Physical Chemistry*, (Goel Publishing House- Meerut, 2008).

Reference Book(s)

1. Viswanathan, B., Raghavan, P. S. *Practical Physical Chemistry* (Viva Books Private Limited, 2008).
2. Gurdeep, R. *Advanced Practical Inorganic Chemistry*, (Krishna Prakashan, 2013).

Volumetric estimation of iron and copper, determination of water of crystallization in a molecule of Hydrated Mohr's salt, estimation of total Hardness of water.

Unit 2

Detection of N, S, and halogens in organic compounds, preparation of suitable derivatives of functional groups and determination of mp/bp

Unit 3

One step organic preparation using common organic reactions such as nitration, acetylation, benzoylation, diazo-coupling etc. **Text Book(s)**

1. Mendham, J., Denney, R. C., Barnes, J. D., Thomas, M. and Sivasankar, B. *Vogel's Quantitative Chemical Analysis*, 6th Edn., (Pearson Education, 2009).
2. Furniss, B. S., Ford, A. J. H., Smith, P. W. H. and Tatchell, A., R. *Vogel's Textbook of Practical Organic Chemistry*, 5th Edn., (John Wiley, 1989).

Reference Book(s)

1. Vishnoi, R. *Advanced Practical Organic Chemistry*, 2nd Revised Edn., (Vikas Publisher, 2007).
2. Gurdeep, R. *Advanced Practical Inorganic Chemistry*, (Krishna Prakashan, 2013).

Course Content:**Unit 1**

Inorganic: Inorganic preparations, Gravimetric estimation of copper and Nickel, Paper chromatographic separation of Ag(I), Hg(II) and Pb(II) ions.

Unit 2

Organic: Qualitative Analysis of solid and liquid organic compounds containing one or more functional groups.

Unit 3

Two step organic preparation using common reagents such as Benzil-Benzilic acid rearrangement, Beckman rearrangement etc.

Unit 4

Physical: Rate constant at elevated temperatures, energy of activation, Polarimetry, Partition function, Critical solution temperature etc.

Text Book(s)

1. Mendham, J., Danney, R. C., Barnes, J. D. and Thomas, M. *Vogel's Textbook of Quantitative Chemical Analysis* (Peterson Education, 2004).
2. Viswanathan, B. and Raghavan, P. S. *Practical Physical Chemistry* (Viva Books Pvt. Ltd., 2005).

Reference Book(s)

1. Furniss, B. S., Ford, A. J. H., Smith, P. W. H. and Tatchell, A., R. *Vogel's Textbook of Practical Organic Chemistry*, 5th Edn., (John Wiley, 1989).
2. Gurdeep, R. *Advanced Practical Inorganic Chemistry*, (Krishna Prakashan, 2013).

Course Content:**Unit 1**

Computational practical

1. DOS, WINDOWS and UNIX operating systems **Unit**

2

1. Programming with FORTRAN77

Unit 3

1. Numerical methods in chemistry (using MS EXCEL)
2. Generation of an EXCEL chart to display the variation of the H_{1s} radial function with radial distance from the nucleus
3. Generation of an EXCEL chart to display the variation of the H_{2s} radial function with radial distance from the nucleus
4. Generation of an EXCEL chart to display the variation of the H_{2p} radial function with radial distance from the nucleus
5. EXCEL charts for the hydrogenic radial distribution functions

Unit 4

1. Generation of the numerical radial wave function for the helium atom "1s' atomic orbital.
2. Generation of the numerical radial wave functions Li_{1s} and Li_{2s} orbitals etc.

Unit 5

Quantum Chemical Calculations with GAUSSIAN and GAMESS

Text Book(s)

1. Balagurusamy, E. *Numerical Methods*, (Tata McGraw-Hill Publishing Company Limited, 2002).
2. Billo, E. J. *Excel for Chemists: A Comprehensive Guide*, (Willy-VCH, 2001).

Reference Book(s)

1. Quinn, C. M. *Computational Quantum Chemistry: An Interactive Guide to Basis Set Theory*, (Academic Press, 2002).

Unit 1

Separation techniques of organic compounds and their spectroscopic identification.

Experiments involving the separation and purification of organic compounds from a mixture, using chromatographic techniques, steam distillation, fractional crystallization and sublimation.

Unit 2

Synthesis of organic compounds using common reagents: At least eight preparation (involving two or more than two steps) involving the following representative reactions: (a) Oxidation of alcohol, (b) Reduction of carbonyl group, (c) Nucleophilic substitution, (d) Cycloaddition reaction, (e) Condensation reaction, (f) Aromatic electrophilic substitution, (g) Preparation of dyes, (h) Heterocyclic synthesis, (i) Solid phase synthesis etc.

Unit 3

Natural product extraction: Caffeine, Nicotine, Carotenoides etc.

Unit 4

Estimation of glucose, acetic acid in vinegar, -OH groups etc.

Unit 5

Determination of acid value and saponification value of fat/ oil.

Unit 6

Green experiments

Text Book(s)

1. Pasto, D., Johnson and Miller, M. *Experiments and Techniques in Organic Chemistry*, (Prentice Hall, 1992).
2. Williamson, K. L. *Macroscale and Microscale Organic Experiments*, (D. C. Heath & Company, 1999).

Reference Book(s)

1. Furniss, B. S., Ford, A. J. H., Smith, P. W. H. and Tatchell, A. R. *Vogel's Textbook of Practical Organic Chemistry*, 5th Edn., (Wiley, 1989).

Unit 1

Quantitative estimation involving volumetric (redox and complexometry), gravimetric and spectrophotometric methods of analysis of constituents in three component mixtures, alloys and minerals.

Unit 2

Synthesis and characterization of inorganic compounds, including those involving green synthetic methodology: Characterization includes elemental analysis, studies by IR, electronic spectra, magnetic susceptibility, conductance measurements, cyclic voltammetry. TG, DSC.

Text Book(s)

1. Mendham, J., Denney, R. C., Barnes, J. D., Thomas, M. and Sivasankar, B. *Vogel's Quantitative Chemical Analysis*, 6th Edn., (Pearson Education, 2009).
2. Marr, G. and Rockett, B. W. *Practical Inorganic Chemistry*, (Van Nostrand, 1972).

Reference Book(s)

1. Wollins, J. D. *Inorganic Experiments*, 3rd Edn., (VCH, 1994).
2. Parshall, G. W. (Ed. in Chief). *Inorganic Synthesis, Vol. 15*, (McGraw Hill, 1974).

Unit 1

Purification of chemicals and calibration of analytical instruments; Error analysis- primary and secondary data, accuracy and precision, averaging of data, types of experimental error, significant figures, estimation and representation of error, and minimization of errors; Handling of basic instruments, e.g., potentiometer, conductivity meter, spectrophotometer, etc., through three basic experiments.

Unit 2

Four minor experiments chosen from: Kinetics by spectrophotometry, polarimetry and conductometry, Relative strength of two acids by conductance, Interfacial tension between two liquids by Tensiometer, Determination of a weak acid and a strong acid in mixture by potentiometry, Study of liquid-liquid phase diagram, Determination of fluoride by ion selective electrode, nitrate spectrophotometry, Determination of average molecular weight of a polymer by viscometry, etc.

Unit 3

Four major experiments chosen from: Study of non-Newtonian polymer solutions by Brookfield viscometer, Study of excess adiabatic compressibility of binary system by ultrasonic interferometry, Simultaneous determination of CMC and partition equilibrium constant by spectroscopic method, Kinetics of the catalytic decomposition of H_2O_2 by manganese (IV) oxide, Determination of CMC by Du Nouy Tensiometry, Micellar catalysis by spectroscopy, Determination of pK_a by spectroscopy, Determination of stoichiometry and the stability constant of the complex formation, Study of pseudo-ternary phase diagram of oil-water-(surfactant-cosurfactant) system, Determination of activation energy of reaction by polarometry, Preparation and characterization of nanoparticles, etc.

Text Book(s)

1. Viswanathan, B. and Raghavan, P. S. *Practical Physical Chemistry*, (Viva Books Pvt. Ltd., 2005).
2. James, A. M. and Prichard, F. E. *Practical Physical Chemistry*, 3rd Edn., (Longman, 1974).

Reference Book(s)

1. Jadaav, J. B. *Advanced Practical Physical Chemistry*, (Krishna Prakashan, 2015).
2. Garland, G. W., Nibler, J. W. and Shoemaker, D. P. *Experiments in Physical Chemistry*, 7th Edn., (McGraw- Hill, 2008).

Course outcomes:

On completion of this course the students will be able to understand:

CO1: Instrumentation technique of various analytical tools like XRD, AAS, cyclic voltammetry, chromatography, optical and electronic microscopy

CO2: Basic principles of those instrumentation techniques

CO3: Application of analytical tools (XRD, SEM, TEM, TGA, AAS, ICP-OES) in characterization and elemental detection of chemical compounds: solids (crystalline, amorphous, nanomaterials), liquids and gases.

CO4: Application of radiochemical techniques in chemical reactions

CO5: Electrochemical techniques for understanding electron transfer reaction mechanism, fuel cell application, Li-ion battery

Course Content:**Unit 1****[4 Lectures]**

X-ray methods: X-ray diffraction, X-ray fluorescence and X-ray absorption and X-ray emission spectroscopy.

Unit 2**[4 Lectures]**

Thermoanalytical methods: Thermo gravimetric analysis, differential thermal analysis and differential scanning calorimetry.

Unit 3**[6 Lectures]**

Electrochemical methods: Coulometry, Polarography, anode-stripping voltammetry, pulse techniques, cyclic voltammetry, electrogravimetry, spectroelectrochemistry.

Unit 4**[5 Lectures]**

Chromatographic methods: Adsorption, liquid-liquid partition, ion-exchange, paper and thin-layer chromatography, HPLC, gel permeation chromatography and gas chromatography, HPTLC, Flash chromatography.

Unit 5**[4 Lectures]**

Radiochemical methods: Tracers in chemical analysis, isotopic exchange, isotopic dilution technique, labeling experiments in studying reaction mechanism.

Unit 6**[8 Lectures]**

Optical microscopy: Optical Rotatory Dispersion and Circular Dichroism: Definition, Deduction of absolute configuration, octane rule for ketones.

Transmission electron microscopy (TEM) and Scanning electron microscopy (SEM).

Unit 7

[5 Lectures]

Atomic absorption spectroscopy: Inductively coupled Plasma- mass spectroscopy (ICPMS), ICP-AES (Atomic Emission Spectroscopy).

Text Book(s)

1. Drago, R. S. *Physical Methods in Chemistry*, (Saunders College Publishing, 1992).
2. Hollas, J. M. *Modern Spectroscopy*, (John Wiley, 1996).

Reference Book(s)

1. Willard, H. H. *Instrumental Methods of Analysis*, (East West Press, 1998).
2. Bard, A. J. and Faulkner, L. R. *Electrochemical Methods, Fundamentals and Applications*, (John Wiley, 2000).

CI 216

Basic Analytical Chemistry

L 3 T 0 P 0 CR 3

Learning outcomes:

After completion of the course, the learner shall be able to learn:

CO1: The method of sampling and the presentation of experimental data

CO2: Calculation of characteristic parameters of samples like soil, water, food, cosmetics etc.

CO3: Use of techniques like chromatography, UV-Vis spectroscopy, flamephotometry in sample analysis

Course Content:

Unit 1

[6 Lectures]

Introduction to Analytical Chemistry and its interdisciplinary nature, concept of sampling, importance of accuracy, precision and sources of error in analytical measurements, presentation of experimental data and results, from the point of view of significant figures.

Unit 2

[5 Lectures]

Analysis of soil: composition of soil, concept of pH and pH measurement, complexometric titrations, chelation, chelating agents, use of indicators, determination of pH of soil samples, estimation of Calcium and Magnesium ions as Calcium carbonate by complexometric titration, analysis of Na/K/N contents, clay, porosity and soil density.

Unit 3

[5 Lectures]

Analysis of water: Definition of pure water, sources responsible for contaminating water, water sampling methods, water purification methods, determination of pH, acidity and alkalinity of a water sample, determination of dissolved oxygen (DO) of a water sample, analysis of total hardness, analysis of total suspended solid, analysis of total dissolved solid, analysis of oil & grease in water.

Unit 4

[4 Lectures]

Analysis of food products: nutritional value of foods, idea about food processing and food preservations and adulteration, identification of adulterants in some common food items like coffee powder, asafoetida, chilli powder, turmeric powder, coriander powder and pulses, etc.; analysis of preservatives and colouring matter.

Unit 5

[4 Lectures]

Chromatography: Definition, general introduction on principles of chromatography, paper chromatography, TLC etc.; paper chromatographic separation of mixture of metal ion (Fe^{3+} and Al^{3+}), comparison of paint samples by TLC method; column, ion-exchange chromatography etc., determination of ion exchange capacity of anion / cation exchange resin (using batch procedure if use of column is not feasible).

Unit 6

[4 Lectures]

Analysis of cosmetics: Major and minor constituents and their function; analysis of deodorants and antiperspirants, Al, Zn, boric acid, chloride, sulphate; determination of constituents of talcum powder: Magnesium oxide, Calcium oxide, Zinc oxide and Calcium carbonate by complexometric titration.

Unit 7

[2 Lectures]

Applications: to study the use of phenolphthalein in trap case, to analyze arson accelerants; to carry out analysis of gasoline.

Unit 8

[6 Lectures]

Instrumental demonstrations: Estimation of macro nutrients: Potassium, Calcium, Magnesium in soil samples by flame photometry, Spectrophotometric determination of Iron in Vitamin / Dietary Tablets, Spectrophotometric Identification and Determination of Caffeine and Benzoic Acid in Soft Drink.

Text Book(s)

1. Day, R. A. and Underwood, A. L. *Quantitative Analysis*, 6th Edn., (Prentice Hall of India, 1991).
2. Skoog, D. A., Holler F. J. and Nieman, T. A. *Principles of Instrumental Analysis*, 6th Edn., (Cengage Learning India Ed, 2014).

3. Skoog, D. A.; West, D. M. and Holler, F. J. *Fundamentals of Analytical Chemistry*, 9th Edn., (Saunders College Publishing, Fort Worth, 2013).
4. Svehla, G. and Sivasankar, B. *Vogel's Qualitative Inorganic Analysis*, 7th Edn., (Pearson Education, 2012).
5. Mendham, J., Denney, R. C., Barnes, J. D., Thomas, M. and Sivasankar, B. *Vogel's Quantitative Chemical Analysis*, 6th Edn., (Pearson Education, 2009).

Reference Book(s)

1. Robinson, J.W. *Undergraduate Instrumental Analysis* 7th Edn., (Marcel Dekker, Inc., New York 2014).
2. Dean, J. A. *Analytical Chemistry Notebook*, 2nd Edn., (McGraw Hill, 2004).
3. Swaddle, T. W., *Applied Inorganic Chemistry*, (University of Calgary Press, 1990).

CI 314

Seminar

L 1 T 0 P 0 CR 1

Presentation by students on chosen topics in the consultation with the course instructor.

3 Course outcomes:

On completion of this course, the students will be able to understand:

C01: Basic principles of the techniques generally involved in chemical processing in Industry

C02: Types of equipment needed in chemical industry

C03: Exploration of societal and technological issues from a chemical perspective **Course**

Content:**Unit 1****[20 Lectures]**

Chemical Technology: Basic principles of distillation, solvent extraction, solid-liquid leaching and liquid-liquid extraction, separation by absorption and adsorption. An introduction into the scope of different types of equipment needed in chemical technology, including reactors, distillation columns, extruders, pumps, mills, emulgators.

Scaling up operations in chemical industry. Introduction to clean technology.

Unit 2**[16 Lectures]**

Exploration of societal and technological issues from a chemical perspective. Chemical and scientific literacy as a means to better understand topics like air and water (and the trace materials found in them that are referred to as pollutants), energy from natural sources (i.e. solar and renewable forms), from fossil fuels and from nuclear fission, materials like plastics and polymers and their natural analogues, proteins and nucleic acids, and molecular reactivity and interconversions from simple examples like combustion to complex instances like genetic engineering and the manufacture of drugs. Adverse effects of pesticides, chemical fertiliser, growth hormones and use of aromatic solvents.

Text Book(s)

1. Hill, J. W., McCreary T. W. and Kolb, D. K. *Chemistry for changing times*, 13th Edn., (Prentice Hall, 2012)

Course outcomes:

After completion of the course, the learner shall be able to learn:

CO1: The basics of unit operations involved in different industrial processing.

CO2: Processes involved in different industries like oil, petrochemical, coal, agrochemical, cement, tea industries.

Course Content:**Unit 1** [6 Lectures]

Unit operations - distillation, extraction, leaching and drying, unit process in organic synthesis - sulfonation, chlorination, nitration, oxidation, hydrogenation and hydrolysis.

Unit 2 [2 Lectures]

Process water, DM water, steam, industrial gases.

Unit 3 [4 Lectures]

Petroleum: Origin and history of petroleum, exploration, reservoir conditions, core, formation water, production, produced water, secondary enhanced oil recovery, drilling fluid, oil-field chemicals, tertiary enhanced oil recovery, transportation of petroleum.

Unit 4 [4 Lectures]

Petrochemicals: refining, composition of petroleum, hydrotreating, cracking of oil, reforming, isomerization, unleaded oil, cracking of natural gas, petrochemicals.

Unit 5 [4 Lectures]

Coal: origin and classification of coal, desulphurization, production of coal chemicals.

Unit 6 [4 Lectures]

Agrochemicals: production of ethanol and methanol, cellulosic products - pulp & paper.

Unit 7 [4 Lectures]

Tea industry - processing of tea, natural fiber- eri and muga production and processing.

Unit 8

[4 Lectures]

Polymers: raw materials, polymer processing, paints, rubber.

Unit 9

[4 Lectures]

Cement – production, various grades of cement, analysis and testing of cement Fertilizer - raw materials and process, sulfuric acid, iron and steel – various grades of products, glass and ceramics, dyes – raw materials and process, dyeing, detergents – raw materials, production, specification and detergency, chlor-alkali industry, electrochemical industry, pharmaceutical industry, fats and oils, fat hardening. Statistical methods for analysis of quality of product, hazards and risk analysis of industry, pollution of air, water and soil, remediation.

Text Book(s)

1. Heaton, A. *The Chemical Industry*, 2nd Edn., (Blackie Academic, 1996).
2. Thompson, R. *Industrial Inorganic Chemicals: Production and Uses* (Royal Soc. of Chem., 1995).

Reference Book(s)

1. Kent, J. A. *Kent and Riegel's Handbook of Industrial Chemistry and Biotechnology*, (Springer, 2010).
2. Speight, J. G. *The Chemistry and Technology of Petroleum*, 5th Edn., (Dekker, 2014).
3. Dawe, R. A. *Modern Petroleum Technology, Vol. 1* (Upstream), 6th Edn., (John Wiley., 2002).
4. Lucas, A. G. *Modern Petroleum Technology, Vol. 2* (Downstream), 6th Edn., (John Wiley., 2002).

Course outcomes:

After completion of the course, the learner shall be able to understand:

CO1: Basic concepts of polymers

CO2: Polymerization techniques and characterization of polymers

CO3: Molecular weight and structure property relationship

CO4: Properties of some important polymers

Course Content:**Unit 1****[6 Lectures]**

Introduction: Historical background, basic nature and classification, importance of polymers as a class of material, polymer raw materials.

Unit 2**[12 Lectures]**

Polymerization techniques: Special features of polymerization, step polymerization, radical chain polymerization, living and non-living chain polymerization, co-ordination polymerization, co-polymerization, ionic polymerization, ring opening polymerization, characterization of polymers, GPC, Spectroscopy of polymer, rheology.

Unit 3**[8 Lectures]**

Structure-property relationship: Stereochemistry of polymers, modification of polymers, cross-linking, polymer architecture, polymer processing and fabrication, polymer composites.

Unit 4**[8 Lectures]**

Natural and synthetic polymers: rubber, natural fibers, silk fibers, PS, Nylon, etc.

Applications of polymers: Applications and future prospects.

Text Book(s)

1. Gowarikar, V.R; Viswanathan, N.V. and Sreedhar, J. *Polymer Science* (Wiley Eastern Limited, 1986).
2. Misra, G. S. *Introductory Polymer Chemistry* (Wiley Eastern Limited, 1993).

Reference Book(s)

1. Sperling, L.H. *Introduction to Physical Polymer Science* (Wiley-Interscience, 1986).
2. Odian, G. *Principles of Polymerization* (Wiley, 2004.)
3. Sun, S. F. *Physical Chemistry of Macromolecules*, 2nd Edn., (Wiley, 2004).