

<b>JSS Science and Technology University, Mysuru</b>		
<b>Course Code</b>	<b>Course Title</b>	<b>Teaching Hours</b>
	<b>FUNDAMENTALS OF CHEMICAL ANALYSIS</b>	52 Hours
<b>COURSE ASSESSMENT METHOD:</b>		
<ul style="list-style-type: none"> <li>• Internal Assessment Marks: 50</li> <li>• Semester End Exam [ 100 Marks, 3 Hours]</li> </ul>		
<b>COURSE OUTCOMES:</b>		
<p>Upon successful completion of this course, students will be able to,</p> <p>CO1 : Understand the basics of analysis of experimental data  CO2 : Understand the basic chromatographic concepts  CO3 : Understand the mechanism of basic organic reactions  CO4 : Understand the concept of bonds and theory of acids and bases  CO5 : to understand the basic of chemical thermodynamics and kinetics</p>		
<b>UNIT:1 – 10 Hours</b>		
<p>Analytical Chemistry: Analysis, determination and measurement. Techniques, methods, procedures and protocols. Classifying analytical techniques. selecting an analytical method - accuracy, precision, sensitivity, selectivity, robustness and ruggedness. Scale of operation, equipment, time and cost. Making the final choice</p> <p>Errors and treatment of analytical data: Limitations of analytical methods – Error: determinate and indeterminate errors, minimization of errors. Accuracy and precision, distribution of random errors, the normal error curve. Statistical treatment of finite samples - measures of central tendency and variability: mean, median, range, standard deviation and variance. Student's t-test, confidence interval of mean. Criteria for the rejection of an observation - Q-test.</p>		
<b>UNIT:2 – 10 Hours</b>		
<p>Chromatography: Definition, principles and mechanism of separation, classification of chromatographic techniques. General descriptions of column chromatography - frontal analysis, displacement analysis and elution analysis. General theory of column chromatography: characterizing a chromatogram - retention time, retention volume and</p>		

baseline width. Chromatographic resolution, capacity factor, column selectivity. Column efficiency - band broadening - rate theory and plate theory. Peak capacity, non ideal behavior.

**UNIT:3 -**

**10**

**Hours**

Basics of organic reactions: Meaning and importance of reaction mechanism, classification and examples for each class.

Aliphatic substitution reactions:

Nucleophilic substitution reactions: Kinetics, mechanism and stereochemical factors affecting the rate of reactions, Neighbouring group participation.

Electrophilic substitution reactions:  $S_E^1$  and  $S_E^2$  reactions

Aromatic substitution reactions:

Nucleophilic substitution reactions:  $S_N^1$ ,  $S_N^2$  and benzyne mechanism, Bucherer reaction.

Electrophilic substitution reactions: Mechanism of Friedel-Crafts alkylation and acylation, Mannich reaction, chloromethylation, Vilsmeier-Haack reaction.

**UNIT:4 -**

**10 Hours**

Ionic bond: properties of ionic substances, coordination number of an ion, structures of crystal lattices- NaCl, CsCl, ZnS and rutile. Lattice energy- Born Lande equation, Born-Haber cycle, Uses of Born-Haber type of calculations. Ionic radii, factors affecting ionic radii, radius ratio rule, covalent character in ionic bonds, hydration energy and solubility of ionic solids.

Theories of acids and bases – Bronsted and Lewis acids and bases, Lux-Flood theory, gas phase vs solution acidity, solvent leveling effects, hardness and softness, HSAB concept. Symbiosis. Applications of HSAB concept.

**UNIT:5 –**

**12**

**Hours**

Thermodynamics - A brief resume of laws of thermodynamics (First and second laws). Entropy as a measure of unavailable energy. Entropy change during spontaneous process. Helmholtz and Gibbs free energies. Thermodynamic criteria of equilibrium and spontaneity. Variation of free energy with temperature and pressure. Maxwell's relations. Nernst heat theorem and Third law of thermodynamics-calculation of absolute entropies. equation.

Chemical Kinetics - Order, molecularity and reaction rate. Determination of rates and orders-

Differential method and Integration method, isolation method, Half life method and Comparison method. Arrhenius Equation, energy of activation and its experimental determination. Kinetic theory of Collision, Activated complex theory of reaction rate.

**TEXT BOOKS / REFERENCES:**

1. Fundamental of Analytical Chemistry, D.A. Skoog, D.M. West, Holler and Crouch, 8<sup>th</sup> edition, 2005, Saunders College Publishing, New York.
2. Analytical Chemistry, G.D. Christian, 5<sup>th</sup> edition, 2001, John Wiley & Sons, Inc, India.
3. Quantitative Analysis, R.A. Day and A.L. Underwood, 6<sup>th</sup> edition, 1993, Prentice Hall, Inc. New Delhi.
4. Inorganic Chemistry, 3<sup>rd</sup> edition. James E. Huheey, Harper and Row Publishers (1983).
5. Inorganic Chemistry, 3<sup>rd</sup> edition. G.L. Miessler and D.A. Tarr, Pearson Education (2004).
6. Inorganic Chemistry, 4<sup>th</sup> edition. P. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong, Oxford University Press (2004).
7. Inorganic Chemistry, 2<sup>nd</sup> edition. C.E. Housecroft and A.G. Sharpe, Pearson Education Ltd. (2005).
8. Organic Chemistry by Morrison and Boyd, PHI, India.
9. Organic Chemistry by Francis A. Carey Tata Mc Graw Hill publishing company Limited, New Delhi.
10. Advanced organic chemistry by Jerry March, Wiley Eastern.
11. Physical Chemistry-Atkins
12. Principles of physical chemistry - Puri, Sharma and Pathania
13. Principles of Chemical thermodynamics – Glass stone
14. Principles of Chemical Kinetics – Glass stone

**ADDITIONAL LEARNING SOURCES:**

<b>JSS Science and Technology University, Mysuru</b>		
<b>Course Code</b>	<b>Course Title</b>	<b>Teaching Hours</b>
	<b>SEPARATION AND CHARACTERISATION TECHNIQUES</b>	52 Hours
<b>COURSE ASSESSMENT METHOD:</b>		
<ul style="list-style-type: none"> <li>• Internal Assessment Marks: 50</li> <li>• Semester End Exam [ 100 Marks, 3 Hours]</li> </ul>		
<b>COURSE OUTCOMES:</b>		
<p>Upon successful completion of this course, students will be able to,</p> <p>CO1 : to acquire the knowledge about HPLC technique  CO2 : to acquire the knowledge about GC and TLC technique  CO3 : to acquire the knowledge about Ion Exchange Chromatography  CO4 : to understand the concepts of thermal characterization techniques like TGA, DTA, DSC  CO5 : to acquire the basic knowledge about NMR Spectroscopy</p>		
<b>UNIT:1 – 10 Hours</b>		
<p><b>High performance liquid chromatography (HPLC):</b> Principles, instrumentation - columns (analytical and guard columns), stationary phases, mobile phases, choosing a mobile phase, isocratic vs gradient elution, HPLC plumbing, sample introduction. Detectors for HPLC - spectroscopic, electrochemical and others, quantitative applications. Preparative HPLC-Applications.</p>		
<b>UNIT:2 – 10 Hours</b>		
<p><b>Gas chromatography (GC):</b> Principles, instrumentation - mobile phase, chromatographic columns, stationary phases, sample introduction, temperature control, and detectors for gas chromatography. Quantitative and qualitative applications.</p> <p><b>Thin layer chromatography:</b> Principle, apparatus and methodology, applications, HPTLC.</p>		

**UNIT:3 -****10****Hours**

**Ion exchange chromatography (IEC):** Definitions, requirements for ion-exchange resin, synthesis and types of ion-exchange resins, principle, basic features of ion-exchange reactions, resin-properties-ion-exchange capacity, resin selectivity and factors affecting the selectivity, applications of IEC in preparative, purification and recovery processes. IEC with eluent suppressor columns. Single Column Ion Chromatography, Detectors.

**UNIT:4 -****10 Hours**

Instrumental techniques: Thermo gravimetric analysis: Introduction, types of thermo gravimetric analysis, principle and method.

Differential thermal analysis: principle of working, theory and instrumentation, simultaneous DTA-TGA curves, factors affecting results and applications.

Differential scanning calorimetry: principles of working, theory, instrumentation and applications.

**UNIT:5 –****12****Hours****NMR spectroscopy**

General introduction and definition, magnetic properties of nuclei (magnetic moment, g factor) and theory of nuclear resonance. Larmor precession frequency, resonance condition and relaxation processes. Chemical shift: Standards employed in NMR, factors affecting chemical shift, electronegativity, shielding and deshielding mechanism, van der Waals deshielding, H-bonding, diamagnetic and paramagnetic anisotropics. Spin-spin coupling, Geminal, vicinal coupling, chemical shift values and correlation for protons bonded to carbon and other nuclei. NMR instrumentation and sample handling. Equivalence and magnetic equivalence proton exchange reactions, effects of chiral center, complex spin-spin interaction, stereochemistry, hindered rotation, Karplus curve - variation of coupling constants with dihedral angles. Simplification of complex spectra: isotopic substitution, increasing magnetic field strength, double resonance, contact shift reagents, Nuclear Overhauser Effect (NOE).

**TEXT BOOKS / REFERENCES:**

1. Fundamental of Analytical Chemistry, D.A. Skoog, D.M. West, Holler and Crouch 8<sup>th</sup> edition, 2005, Saunders College Publishing, New York.
2. Analytical Chemistry, G.D. Christian, 5<sup>th</sup> edition, 2001 John Wiley & Sons, Inc. India.
3. Quantitative Analysis, R.A. Day and A.L. Underwood, 6<sup>th</sup> edition, 1993 Prentice Hall, Inc. New Delhi.

4. Analytical Chemistry Principles, John H. Kennedy, 2<sup>nd</sup> edition, Saunders College Publishing, California, 1990.
5. Instrumental Method of Analysis, W.M. Dean and Settle, 7<sup>th</sup> edition, 1986, CBS Publishers, New Delhi.
6. Modern Analytical Chemistry, David Harvey, McGraw Hill, New Delhi, 2000.
7. Spectroscopy by P.S Kalsi.
8. Organic Spectroscopy by Warren.

**ADDITIONAL LEARNING SOURCES:**

**JSS Science and Technology University, Mysuru**

Course Code	Course Title	Teaching Hours
	<b>ADVANCED CO-ORDINATION CHEMISTRY</b>	52 Hours

**COURSE ASSESSMENT METHOD:**

- Internal Assessment Marks: 50
- Semester End Exam [ 100 Marks, 3 Hours]

**COURSE OUTCOMES:**

Upon successful completion of this course, students will be able to,

CO1 : Understands the stability of coordination compounds

CO2 : Understands the chemical equilibrium in coordination compounds

CO3 : Understanding the reaction mechanism of co-ordination compounds

CO4 : Understanding the basics of metal-ligand bonding in co-ordination compounds

CO5 : Understand the characterization tools of coordination compounds

**UNIT-I**

**Preparation of coordination compounds:** Introduction, Preparative methods - simple addition reactions, substitution reactions, oxidation-reduction reactions, thermal dissociation reactions, reactions of coordinated ligands.

**Stability of coordination compounds:** Introduction, trends in stepwise stability constants, factors influencing the stability of metal complexes with reference to the nature of metal ion and ligands, the Irving-William series, chelate effect.

**Determination of stability constants:** Theoretical aspects of determination of stability constants of metal complexes by spectrophotometric and pH metric.

## UNIT-II

**Metal-Ligand equilibria in solution-** Step-wise and overall formation constant and their Relationship, trends in step-wise constant, kinetic and thermodynamic stability of metal complexes, factors affecting the stability of metal complexes with reference to the nature of the metal ion and ligand, chelate effect.

**Structure and bonding-** Structure and bonding in hydride, dihydrogen, dioxygen, isocyanide, CO, NO, N<sub>2</sub> and tertiary phosphine metal complexes.

## UNIT - III

**Reaction Mechanisms in Transition Metal Complexes:** Energy profile of a reaction, inert and labile complexes, kinetics of octahedral substitution and mechanistic aspects. Acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism and evidences in its favour. Anation reactions, reactions without M-L bond cleavage.

**Substitution reactions in square planar complexes:** Trans effect, mechanisms of substitution.

**Electron transfer reactions:** inner sphere and outer sphere reactions, the Marcus theory, complimentary and non-complimentary reactions.

## UNIT - IV

**Metal- ligand bonding-**Crystal field theory, salient features, spectrochemical series, splitting of d-orbitals in tetragonal, square planar, and octahedral geometry. Distortion of octahedral complex, CFSE and their uses, factors affecting CFSE, Applications and limitations of CFT. CFT- colours of transition metal complexes, magnetic properties of metal complexes, experimental evidence for metal-ligand covalent bonding in complexes. Ligand Field Theory, MO theory: tetrahedral and octahedral complexes (without  $\pi$ -bonding).

## UNIT-V

**Characterization Technique:**

**IR Spectra:** Identification of functional groups - alkenes, aromatics, carbonyl compounds (aldehydes and ketones, esters and lactones), halogen compounds, sulphur and phosphorus compounds, amides, lactams, amino acids and amines. Applications of IR spectroscopy.

**NMR Spectra:** Chemical shift, Standards employed in NMR, factors affecting chemical shift, electronegativity, shielding and deshielding mechanism, van der Waals deshielding, H-bonding, diamagnetic and paramagnetic anisotropics. Spin-spin coupling, Geminal, vicinal coupling, chemical shift values and correlation for protons bonded to carbon and other nuclei.

**Mass spectra:** molecular ion, base peak, meta-stable peak. Mass spectral fragmentation of organic compounds (acids, esters, hydrocarbons, halogenated hydrocarbons, alcohols, carbonyl compounds, amines, ethers and heterocyclic compounds).

#### **TEXT BOOKS / REFERENCES:**

##### **REFERENCES**

1. Basic Inorganic Chemistry- F. A. Cotton, G. Wilkinson and P. L. Gaus; John Wiley and sons. Inc, 6th edition (1999).
2. Chemistry of elements- N. N. Greenwood and A. E. Earnshaw, Butterworth Heinemann (1997).
3. Inorganic Chemistry IV edition; J. E. Huheey, E. A. Keiter and R. L. Keiter, Addison; Wesley (1993).
4. Inorganic Chemistry, II edition, D. F. Shriver, P. W. Atkins and C. H. Langford, ELBS; Oxford University Press, 1994.
5. Inorganic Electronic spectroscopy, A. B. P. Lever, Elsevier. (1968).
6. Magnetochemistry, R.L. Carlin, Springer Verlag.
7. Electronic Absorption Spectroscopy and related Techniques, D. N. Sathyanarayana, University Press (2001).
8. Inorganic Chemistry A Unified Approach by W. W. Porterfield, Elsevier 2005 2nd edition.
9. Textbook of inorganic chemistry by G. S. Sodhi, Viva books Pvt. Ltd (2011).
17. A Guide Book to Mechanism in Organic Chemistry by Petersykes
18. Text book of Organic Chemistry by P.S. Kalsi.
19. F.A. Carey and Sundberg, Advanced Organic Chemistry – Part A & B, 3rd edition, Plenum Press, New York, 1990.
20. S.K. Ghosh, Advanced General Organic Chemistry, Book and Alleied (P) Ltd, 1998.

#### **ADDITIONAL LEARNING SOURCES:**



