

DR BR AMBEDKAR OPEN UNIVERSITY – HYDERABAD

DEPARTMENT OF CHEMISTRY

PRE-Ph.D CHEMISTRY SYLLABUS

INORGANIC CHEMISTRY

Guide: Dr. K. Prameela

Research Scholar : Smt. Valli Sowbhagyam

**Unit-1: UV-Visible Spectroscopy and IR Spectroscopy - Raman Spectroscopy**

**UV-Visible Spectroscopy**

Introduction; Absorption Laws; Formation of Absorption bands ;Theory of Electronic Spectroscopy; Theory of Electronic Transitions; Chromophore concept; Auxochrome; Types of Absorption bands; Solvent effect; Instrumentation; Woodward – Fischer rules for calculating absorption maxima in dienes and  $\alpha,\beta$ -unsaturated carbonyl compounds; Steric hindrances and co-planarity; Estimation of ligand-metal ratio in complexes; Applications.

**IR Spectroscopy - Raman Spectroscopy**

Infrared and Raman Spectroscopy Conditions for Infrared and Raman Spectroscopies – Structure Fitting. Determination of Coordination Sites and Linkage Isomers( $\text{NO}_2^-$ ,  $\text{SCN}^-$ ), Assigning Denticity of Ligands ( $\text{SO}_4^{2-}$ ,  $\text{CO}_3^{2-}$ ), Prediction of Diagnostic Fundamentals in Isomers of Metal Complexes and Distinguishing Isomers of Metal Complexes. Effect of Coordination on Ligand Vibrations: Examples involving Mono, Bi and/or Polydentate Ligands of Oxygen, Sulfur, Nitrogen, Phosphorous, Carbon and Halogen Donors ( $\text{NH}_3$ ,  $\text{H}_2\text{O}$ , Glycine,  $\text{PPh}_3$ , 2,2'-Bipy, 1,10-Phen, Carbonyl and halides). Raman effect and molecular structure-  $\text{CO}$ ,  $\text{HCN}$ ,  $\text{CO}_2$ ,  $\text{N}_2\text{O}$ ,  $\text{H}_2\text{O}$ . Principles of Resonance Raman Spectroscopy. Application of Resonance Raman Spectroscopy to Structural Elucidation of the active Sites of Heme and Non-Heme Oxygen Carriers.

**Unit-2: Mass Spectrometry and Advanced NMR Spectroscopy:-**

Advanced Mass spectrometry Quadruple analysers, Ion traps. Time of flight mass spectrometry. Mass Spectrometry/Mass Spectrometry Tandem Mass Spectrometry. Ion cyclotron resonance spectrometers and Ion traps for MS/MS. Quantitative mass spectrometry: Introduction, principle, calibration and internal standards. Hyphenated techniques: GC-MS: Principle, instrumentation, Interfaces, Mass analyzer, Mass chromatogram, Applications. Analysis of metabolite of drug Imipramine GC-FT-IR: Principle, Instrumentation and Applications LC-MS: Principle, Instrumentation, Interfaces and Applications. LC-MS-MS : Principle, Instrumentation, Interfaces and Applications. ICP-MS: Instrumentation, principles, Quantitative analysis and applications.

**NMR Spectroscopy:-**

$^1\text{H}$  NMR and  $^{13}\text{C}$  NMR spectroscopy: introduction, principle, instrumentation and applications of  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR Spectroscopy. First order, non first order spectra eg. AX, AX<sub>3</sub>, A<sub>2</sub>X<sub>3</sub>, AMX, AB and ABC, Nuclear overhauser enhancement (NOE).

**Unit-3: CHROMATOGRAPHY**

**Gas Chromatography:**

Introduction and importance; Instrumentation - sample injection, carrier gas, capillary columns, bonded phase, dual detection; Temperature programming; Commercial Gas Chromatograms; Qualitative analysis; Quantitative analysis; Applications.

*Prameela*

## HPLC:

Instrumentation: Sample injection, Detectors, Qualitative analysis; Quantitative analysis; Applications.

### Unit – 4: Co-ordination chemistry: Theory, structure and reaction mechanism

Werner's theory Representative ligands, Nomenclature; Constitution and geometry- Coordination number, polymetallic complexes; Isomerism and Chirality- Square planar, Tetrahedral and octahedral complexes, ligand chirality Metal ligand Bonding: Crystal Field Theory (CFT) for bonding in transition metal complexes, crystal field splitting of "d"- orbitals in octahedral, tetrahedral, tetragonal and square planar fields. Crystal Field Stabilization energy (CFSE) and its calculation in six and four coordinated complexes, Spectrochemical series with reference to ligands and metal ions. Factors affecting the magnitude of  $\Delta_o$  in octahedral complexes, Jahn-Teller effect and its consequences.

Thermodynamic origin- Step-wise and overall stability of the complex, Chelate, macrocyclic and cryptate effects; Determination of stability constant of a complex using pH metry, spectrophotometry and polarographic techniques. Magneto Chemistry: diamagnetism para-magnetism, ferro- and anti-ferromagnetism, susceptibility, magnetic moment, super exchange, Curie-Weiss law.

### Unit – 5: Electronic spectroscopy of transition metal complexes and Bioinorganic chemistry

Energy levels in an atom, microstates – calculation of microstates; Spectroscopic states – coupling of orbital angular momenta and spin angular momenta; Spin – orbit coupling (R-S coupling) Derivation of term symbols for  $p^2$  and  $d^2$  configurations. Determination of ground state terms – Hund's Rules; Hole formalism. Electronic spectra of octahedral and tetrahedral complexes. Nature of electronic spectrum; Laporte orbital and spin selection rules; Transforming spectroscopic terms into Mullikan symbols. Spectra of  $d^1$  to  $d^9$  metal ions/complexes. Orgel diagrams, Tanabe Sugano diagrams and comparison between these diagrams. Charge transfer ( $L \rightarrow M$  and  $M \rightarrow L$ ) spectra in inorganic compounds. Nature of electronic spectra of f-block metal complexes.

Metal ions in Biology, Molecular mechanism of ion transport across membranes; ionophores, photosynthesis, nitrogen fixation, oxygen uptake proteins, cytochromes and ferredoxins.

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Pre - Ph. D

**Syllabus for Ph.D. in the Faculty of Science  
Research Methodology**

Sus: Chemistry

**UNIT-1**

Scientific Method: Meaning and Definition, scientific process and justifying the scientific method. Research Ethics: Definition, principles, general responsibilities and obligations. Identification of Research Problem: Definition of research problem, Selecting the problem, Necessity of Defining problem, various techniques involved in defining a problem. Research methods: Meaning of Research, Objectives of Research, Types of Research, Significance of Research, Research Method versus Research Methodology, Research and Scientific Method, Research Process and Criteria of Good Research. Review of Literature Dimensions of Research: Qualitative and Quantitative research – concept of measurement, causality, generalization, replication. Merging the two approaches. Concept of measurement, scaling, scaling techniques, multidimensional scaling. Research Design: Meaning, Need for Research Design, Feature of a Good Design, Different Research Designs, Experimental - Non Experimental Designs and importance.

**UNIT-2**

Data Collection: Introduction, Experiment and Surveys, Collection of Primary Data, Difference between Questionnaire and Schedule, Some other methods for Data Collection, Collection of Secondary Data and Selection of Appropriate Method for Data Collection. Statistics in Research: Role of Statistics in Research, Measures of Central Tendency, Measures of Dispersion, Measure of Skewness, Kurtosis and Measure of Relationship. Sampling and Statistical Inference: Parameter and Statistic, Sampling and Non Sampling Errors, Sampling Distributions, Statistical Inference, Chi-Square test, t-test, ANOVA, regression and multiple regression analysis, Factor and Principle component analysis.

**UNIT-3**

Hypothesis: formation of Hypothesis, testing of Hypothesis: Basic concepts testing of Hypothesis, Null Hypothesis and Alternative Hypothesis, Type I and Type II Errors, Level of Significance, Test Statistic and Critical Region, Hypothesis for mean, Hypothesis for proportion, Hypothesis testing for variance, Limits of tests of the Hypothesis. Multivariate Techniques for Data interpretation: Characteristics and Applications, Classification of Multivariate Techniques, Path Analysis, Canonical Correlation, Multidimensional Scaling and Latent Structure Analysis. Thesis writing: Significance of Report Writing, Different Steps in writing Report, Types of Research Reports, Mechanics of Writing a Research Report, Precautions for writing Research Reports, Bibliography and References.

**UNIT-4**

Computer Applications: Number system – binary, octal and hexadecimal, base conversion. Logic gates-AND, OR NOT. 2 Data Structure – array, stack (push, pop), queue (inset, delete), linked list-singly, doubly, operating system – definition, types of OS. Use of software – MS office, Power Point, WORD and EXCEL and ACCESS, Computer viruses, Uses of Internet – OERs, Open accesses journals, Journals Data Base, misuse of Internet, Hacking, Field hazards. Instrumentation: Description and principles of (i) Electrophoresis (ii) PCR Machine (iii) Laminar Flow (iv) Ultracentrifuge (v) Autoclave (vi) Light and Electron microscopy, chromatography and HPLC (vii) Fluorescence CPI (viii) AAS (ix) UV – Visible (xi) IR –Raman, Handling of instruments and precautions.

**UNIT-5**

Safety Measures: (i) Lab Safety Measures: Introduction, Code of Conduct – while entering in the lab, while working with the chemicals, while disposal of chemicals, storage and disposal of chemical – aqueous wastes, organic and radioactive wastes. Human contribution to reduce hazardous wastes. (ii) field Safety measures; Food security during field trip/expedition, safety measures during field trip/expedition – self – care, avoid in fields, care from wild animals, hazard warnings, Safety measures during visit to library and villages, first aid in the fields.

## **Syllabus for M.Phil. in the Faculty of Science**

### **Research Methodology**

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