

**Avinashilingam Institute for Home Science and Higher Education for Women**  
 (Deemed-to-be-University under Category A by MHRD, Estd. u/s 3 of the UGC Act 1956)  
 Re-accredited with 'A++' Grade by NAAC, Recognized by UGC u/s 12B  
 Coimbatore 641 043, Tamilnadu, India  
 Department of Chemistry  
 Ph.D – Chemistry (Full time)

**Name of the Scholar : J. Sivasankari Roll No.: 21PHCHF004**

**Name of the Supervisor : Dr. M. Amutha Selvi**

**21PHCH03D - Advanced Co-ordination Chemistry**

(For Ph.D Full Time scholar admitted in January 2022)

**Hours of Instruction per week:4**

**Objectives:**

- To learn the concepts of co-ordination chemistry
- To know the basics of Theories of co-ordination bond
- To understand the role of metals in biological system

**Unit I Bonding in Metal Complexes**

Crystal field theory - splitting of orbitals in octahedral, tetrahedral, square planar, square pyramidal and trigonal bipyramidal fields - Ligand field stabilisation energy –John Teller effect - Evidence for metal ligand overlap.Molecular orbital theory of transition metal complexes-Molecular orbital energy level diagram for octahedral complexes with and without pi-bonding.

Intra ligand & charge transfer transitions (LMCT & MLCT) - Types of  $d^n$  configuration- Term symbols, Orgel and Tanabe-Sugano diagrams - Interpretation of electronic spectra of metal complexes - Racha parameters. **12h**

**Unit II Chemistry of Metals**

A comparative study of complex formation by metal ions – First row transition metal ions in comparison with metal ions of second and third row (co-ordination number, stability and geometry of the complexes) – Metal complexes as imaging agents-Nuclear medicine – Applications of Technetium labeling- Complexes of Lanthanides & Lanthanide shift reagents.

Transition metal ions in biology – Metallobiomolecules - Electron carriers, oxygen carriers, enzymes.Specific examples: Hemoglobin, Myoglobin. Biomaterials – Biological response to biomaterials – Properties of biomaterials – degradative, surface, mechanical and bulk properties. **12h**

**Unit III Synthesis and Mechanism of Metal Complex Formation**

Experimental methods of synthesis and purification of ligands -Schiff's bases and oximes – synthesis and complexation.Synthesis of complexes - Simple and template method of synthesis –reductive ligation using  $LiAlH_4$  or  $NaBH_4$  -Alkyl cobaloximes - Synthesis in inert atmospheric condition- Synthesis involving microwave assisted condition.

Inert and labile complexes - crystal field activation energy – possible mechanisms for ligand replacement reactions. Ligand exchange reactions in octahedral complexes of cobalt (III) and square planar platinum (II) complexes – Trans effect – electron transfer processes. Electron transfer reaction, outer sphere and inner sphere electron transfer, one and two electron transfer reactions, electron transfer through extended bridges, mixed valence compounds, unstable oxidation state. **12h**

#### Unit IV Characterization of the Complexes

Spectral analysis of complexes - NMR, ESR, SEM, UV, IR, TG-DTA, Magnetic properties and kinetics of adsorption. Diffraction studies - Single crystal XRD and powder XRD. Biological activities –docking and DNA binding studies. **12h**

#### Unit V Advanced Inorganic Chemistry

Inorganic frame work materials –Zeolites - Building units, Relation between zeolites structures and applications. Various methods to synthesis metal inorganic frameworks. Polymerization of complexes.

Contrast enhancing agents for medical diagnostics, theory of MRI imaging, Gd based contrast agents-synthesis and structural features; optical contrast agents Ag and AuNPs. Metal complexes for radiotherapy, diagnostic radiopharmaceuticals. Applications of organometallics in medicine and industries **12h**

#### Course outcomes

- Ability to understand the various theories of metal complexes.
- Ability to recognize the chemistry of metals and properties of various biomaterials.
- Able to familiarize the synthesis and mechanism of metal complex Formation.
- Ability to qualitatively analyze the spectral characteristics of complexes.
- Able to know recent applications of coordination complexes.

#### References

1. Advanced Inorganic Chemistry., F. Albert Cotton and Geoffrey Wilkinson., Wiley, John & Sons, Incorporated, 1st Ed. 1962, 6th Ed. 1999.
2. Physical Chemistry., Sibey, Alberty, Bawendi., Wiley Student edition, Fourth edition, 2012.
3. Inorganic Chemistry., Weller, Overton, Rourke, Armstrong., South Asia edition, 6<sup>th</sup> edition.
4. Inorganic chemistry- Principles of structure and reactivity., James E. Huheey, Ellen A. Keiter, Richard L. Keiter, Okhil K. Medhi., Pearson Education, 2009.
5. Bioinorganic Chemistry., K. Hussain Reddy, New Age International Publishers, 2003
6. Principles of Bioinorganic Chemistry., S. J. Lippard and J. M. Berg, University Science Books, Mill Valley, 1994.
7. Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life., W. Kaim and B. Schwederski, John Wiley & Sons Inc., 1994
8. Biomaterials: The Intersection of Biology and Materials Science., J.S. Temenoff, A.G. Mikos., Pearson Education, 2009.
9. Concepts and Models in Inorganic Chemistry., D.E. Douglas, D.H. McDaniel, J.J. Alexander, 3<sup>rd</sup> Ed, 1994.
10. Concise Inorganic Chemistry., J.D. Lee, 5<sup>th</sup> Ed, Wiley, 1999.
11. Structural Methods in Inorganic Chemistry., E.A.V. Ebsworth, 3<sup>rd</sup> Ed., ELBS, 1987.
12. Principles of Organometallic Compounds., C E Coates. M L H Green, P Powell K Wade, Chapman and Hall, 1977.
13. Inorganic Chemistry., M. F. Purcell, J. C. Kotz, Saunder, 1977.
14. Physical Methods in Inorganic Chemistry., R.S. Drago, 3<sup>rd</sup> Ed., Wiley Eastern Company
15. Concepts and Models in Inorganic Chemistry., D.E. Douglas, D.H. McDaniel, J.J. Alexander, 3<sup>rd</sup> Ed. 1994.
16. Mechanism of Inorganic reactions., F. Basolo and R.G. Pearson, New York, Wiley.
17. Introduction to Magnetic Chemistry., A. Earnshaw, Academic Press.

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**Coimbatore 641 043, Tamilnadu, India**  
**Department of Chemistry**  
**Ph.D – Chemistry (Part time)**

**Name of the Scholar** : S.Vinodha **Roll No.:**21PHCHP004  
**Name of the Supervisor** : Dr. Shubashini K.Sripathi

**Hours of Instruction per week:4**  
**21PHCH03E-PHYTOCHEMICAL METHODS AND PAPER MAKING TECHNOLOGY**

(For Ph.D Part Time scholar admitted in January 2022)

**Objectives:**

- To gain knowledge about the Isolation and Purification of natural products.
- To get acquainted with preliminary phytochemical techniques.
- To gain knowledge about spectral characterization of natural products.
- To gain knowledge about pulp and paper making raw materials.
- To get acquainted with kraft and soda recovery cycles.

**Unit - 1**

Isolation and purification of natural products- general methods used for isolation and purification of natural products, super critical fluid extraction. Principle and application of chromatographic techniques such as Column, HPTLC, HPLC, TLC and GC in the isolation and purification of natural products.

**12h**

**Unit - 2**

Preliminary Phytochemical investigation of bioactive phytoconstituents – Alkaloids, Phenolics and Tannins – Color Tests, Fluorescence characteristics – Physical data – TLC analysis.

Spectral characterization of Natural Products- UV Visible, IR, NMR and Mass spectral techniques- Shift reagents in UV.

**12h**

**Unit – 3**

A brief description raw materials, Paper making raw materials, Selection of pulp and paper making raw materials (a) Wood based raw materials (b) Non woody raw materials, Brief description of pulp and paper making process , Description of various grades of pulp and paper, Properties of paper- Alternative raw material for wood pulp and sustainability of raw materials and various paper coating raw materials.

**12h**

**Unit – 4**

Chemical composition of fibrous raw materials, Cellulose – Isolation, structure and chemical properties, Cellulose derivatives – Preparation and end use, Hemicelluloses – Isolation, importance in paper making, reactions during pulping, Lignin-Isolation, structure linkage, physical and chemical properties, Extractives – Isolation and significance in pulp and paper making.

**12h**

## Unit – 5

Kraft and Soda recovery cycles - Quality and concentration of black liquor; Influence of dilution; Composition of black liquor for wood and non-woods- Impact of Black Liquor properties on Evaporator and Recovery Boiler – Black Liquor Combustion: Process chemistry, droplet formation, swelling, char combustion, sulfide reduction and carbon oxidation, entrainment and carryover, potassium enrichment, volatilization of chloride, deposits and boiler plugging.

12h

### Reference Books:

1. Harborne J.B., "Phytochemical Methods", Chapman and Hall, 1998
2. James P. Casey, "Pulp and Paper: Chemistry and Chemical Technology", John Wiley and Sons. 1984
3. Browning B. L. "The Chemistry Of Wood", John Wiley and Sons. 1981
4. Smook G. A. "Handbook for Pulp and Paper Technologies", TAPPI press. 1989

### Course outcomes

- Skills of isolation and purification of natural products
- Knowledge on characterizing natural products
- Knowledge on new materials for paper making, pulp making process and properties of paper
- Understanding of the chemical composition of fibrous new materials
- Understanding of the byproducts of paper making ,blackliquor and its constituents

*Resoualea*