

**ADIKAVI SRI MAHARSHI UNIVERSITY  
RAICHUR**



**SYLLABUS  
DEPARTMENT OF STUDIES IN CHEMISTRY**

**Syllabus for Ph.D Course Work**

**With effect from 2025-26**

# **Department of Studies in Chemistry**

## **Objectives of Chemistry Program**

- To understand the basics of research and its importance
- To know the ethics involved in research and publications
- To revise the applied concepts of chemistry logically with emphasis on practical aspects.
- Developing the analytical skills in various classical and instrumental methods of analysis.
- To impart educational skills and the knowledge in Chemistry to apply it in related areas.
- Improve the communication skills and inspire for future careers in the field of Chemistry.

## **Outcomes of Chemistry Program**

- Students will acquire idea and skills related to research.
- Will get awareness about ethics in research.
- The seminars and interactions will improve the communication skills and confidence.
- Course work will revise the basics as well as in the applied area of chemistry before they take up research

# CHEMISTRY (PhD)

(2020-21)

The Board has amended the Syllabus / Scheme of examination and recommended for implementation from 2020-2021. The following are the papers and scheme of examination proposed by the Board.

1. Ph.D Degree Course work examination

## COURSE STRUCTURE AND SCHEME OF EXAMINATION Ph.D. COURSE WORK IN CHEMISTRY

Paper Code	Paper Title	Contact Hours/ Week & Credits	Internal Assessment Weightage		Semester End Exam Duration(hrs) & Assessment Weightage	Total Marks/Paper
			I test	II test		
CHE RPE-1	Research Publication and Ethics	2h & 2	10%	10%	2h & 40%	50
CHE RM-2	Research Methodology	4h & 4	15%	15%	3h & 70%	100
CHE CP-3	Cognate paper- Selected topics in chemistry	4h & 4	15%	15%	3h & 70%	100
CHE SP-IN-4 (special paper)	Inorganic Chemistry and Nanoscience	4h & 4	15%	15%	3h & 70%	100
CHE SP-PC-4 (special paper)	Physical Chemistry	4h & 4	15%	15%	3h & 70%	100
CHE SP-OC-4 (special paper)	Organic chemistry	4h & 4	15%	15%	3h & 70%	100
CHE SP-CC-4 (special paper)	Chemistry of Coordination Compounds	4h & 4	15%	15%	3h & 70%	100
CHE SP-OM-4 (special paper)	Organometallic Chemistry	4h & 4	15%	15%	3h & 70%	100
<b>Total</b>	<b>4 papers</b>	<b>11h/week, 14 credits</b>				<b>350</b>
<b>Viva-Voce</b>						<b>50</b>

Note: Research methodology, Research Publications and Ethics and cognate subject are compulsory to all the research students. Students can opt anyone of the specialized paper Course- CHE SP-4

## Department of Studies in Chemistry

### Ph.D. Course work

#### Course-I : CHE RPE-1: Research Publication and Ethics

30 hours

2 hrs/week

**Unit-I: RPE 01: PHILOSOPHY AND ETHICS (3 hrs):** Introduction to philosophy: definition, nature and scope, concept, branches. Ethics: definition, moral philosophy, nature of moral judgements and reactions

**RPE 02: SCIENTIFIC CONDUCT (5 hrs):** Ethics with respect to science and research; Intellectual honesty and research : Integrity; Scientific misconducts: Falsification, Fabrication, and Plagiarism (FFP): Redundant publications: duplicate and overlapping publications, salami slicing; Selective reporting and misrepresentation of data

#### **Unit-II: RPE 03: PUBLICATION ETHICS (7 hrs)**

Publication ethics: definition, introduction and importance; Best practices / standards setting initiatives and guidelines: COPE, WAME, etc.; Conflicts of interest; Publication misconduct: definition, concept, problems that lead to unethical behavior and vice versa, types; Violation of publication ethics, authorship and contributorship; Identification of publication misconduct, complaints and appeals; Predatory publishers and journals

### **PRACTICE**

**Unit-III: RPE 04: OPEN ACCESS PUBLISHING (4 hrs):** Open access publications and initiatives; SHERPA/RoMEO online resource to check publisher copyright & self-archiving policies; Software tool to identify predatory publications developed by SPPU; Journal finder / journal suggestion tools viz. JANE, Elsevier Journal Finder, Springer Journal Suggester, etc.

#### **RPE 05: PUBLICATION MISCONDUCT (4 hrs):**

- A. Group Discussions (2 hrs.)-** Subject specific ethical issues, FFP, authorship; Conflicts of interest; Complaints and appeals: examples and fraud from India and abroad
- B. Software tools (2 hrs)-** Use of plagiarism software like Turnitin, Urkund and other open source Software tools

#### **Unit-IV: RPE 06: DATABASES AND RESEARCH METRICS (7hrs)**

- A. Databases (4 hrs):** Indexing databases; Citation databases: Web of Science, Scopus, etc
- B. Research Metrics (3 hrs):** Impact Factor of journal as per Journal Citation Report, SNIP, SJR, IPP, Cite Score; Metrics: h-index, g index, i10 index, altmetrics

**Reference Books:**

- 1) C. R. Kothari, Research Methodology: Methods and Techniques, New Age International Publishers, New Delhi, 2004
- 2) Deepak Chawla and Neena Sodhi, Research Methodology, Concepts and cases, 2<sup>nd</sup> ed., Vikas Publishing House Pvt Ltd., New Delhi, 2015
- 3) Vinayak Bairagi and Mousami V Munot, Research Methodology: A practical and Scientific Approach, CRC Press, New York, 2019
- 4) Comstock Gary, Research Ethics, Cambridge University Press, 2013
- 5) David Bridges, Philosophy in Educational research, Epistemology, Ethics, politics and quality, Springer International Publishing, AG, 2017
- 6) Peter Pruzan, Research Methodology; The Aims, Practices and Ethics of Science, Springer International Publishing, Switzerland, 2016.
- 7) C. George Thomas, Research Methodology and Scientific writing, II Edition, Springer, 2021.

## Department of Studies in Chemistry

### Ph.D. Course work

#### Course-II: CHE RM-2 Research Methodology

48 hours

3hrs/week

##### UNIT 1: Research sources

12 hrs

Selection of research problems and literature survey: primary sources- Journals periodicals, abstracts; Secondary listing of titles, reviews –annual Treatises, serials, monographs and text books, encyclopedia, catalogues, index of tabulated data- Science citation index- Searching the chemical literature-location of journal article- materials on a given topic- information about specific compound- Choosing a problem-abstract of a research paper. Scientific ethics.

Internet: Introduction to internet-web browsers-World Wide Web-Search engines-literature survey in Chemistry-popular website in chemistry-Database in chemistry. usage of packages (e.g. ORIGIN; EXCEL) for data analysis; basics of computer operations; using windows – directory structures – command structure (document preparation, EXCEL, Power Point Presentation); E-Mail: Introduction to e-mail- creating e-mail-Receiving and sending e-mail.

##### UNIT 2 : Research data presentation

12 hrs

Research manuscript preparation Full length research paper, short communication, letters, reviews, popular science articles in magazines, Few case studies with reference to journals and periodicals. Presentation of research papers: Oral and poster presentation in seminars, workshops and conferences etc.. Preparation of synopsis and Thesis, Preparation of research project proposals. Patent: Introduction, patentable subject

##### UNIT 3: Purification and safety measures

12 hrs

Handling of chemicals; hazardous chemicals; air/water sensitive, corrosive, toxic, explosive, carcinogenic and radioactive materials. Safety measures in laboratory, Good laboratory practices (GLP). **Emergency response** : chemical spills, radiation spills, biohazard spills, leaking compressed gas cylinders, fires, medical emergency accident reporting; safety equipments, personal protective equipments, compressed gas safety, safety practices for disposal of broken glass wares.

Purification of compounds: General methods of isolation and purification of chemicals. Solvent extraction both cold and hot methods of crystallization, fractional crystallization, sublimation, Distillation; fractional distillation, distillation under reduced pressure, steam distillation, drying methods of solvents.

#### **UNIT 4:Error Analysis in Chemical Measurements and results**

12 hrs

Classification of errors-Accuracy-Precision-Minimization of errors-Significant figures. Statistical treatment of data: Mean and Standard Deviation-distribution of random and normal errors-Reliability of results- Confidence interval- Comparison of mean results students t-distribution and t- tests-Comparison of mean with expected value, comparison of the results of the two different methods, comparison of precision of two methods- Linear regression, regression line, standard deviation, correlation coefficient – Multiple linear regression (one variable with two other variables).

#### **Reference books:**

- 1) C. R. Kothari, Research Methodology: Methods and Techniques, New Age International Publishers, New Delhi, 2004
- 2) Deepak Chawla and Neena Sodhi, Research Methodology, Concepts and cases, 2<sup>nd</sup> ed., Vikas Publishing House Pvt Ltd., New Delhi, 2015
- 3) Vinayak Bairagi and Mousami V Munot, Research Methodology: A practical and Scientific Approach, CRC Press, New York, 2019
- 4) Comstock Gary, Research Ethics, Cambridge University Press, 2013
- 5) David Bridges, Philosophy in Educational research, Epistemology, Ethics, politics and quality, Springer International Publishing, AG, 2017
- 6) Peter Pruzan, Research Methodology; The Aims, Practices and Ethics of Science, Springer International Publishing, Switzerland, 2016.
- 7) Vogel's Quantitative Inorganic analysis, 7<sup>th</sup> Ed., 2012
- 8) G.D. Christian, Analytical Chemistry, 7<sup>th</sup> Ed., Wiley , 2013
- 9) C. George Thomas, Research Methodology and Scientific writing, II Edition, Springer, 2021.

**Course -III : CHE CP-3 Cognate subject**

**SELECTED TOPICS IN CHEMISTRY**

48 hours

3hrs/week

**UNIT-1 Analytical and spectroscopic technique:**

12 hrs

**Chromatographic technique:** Classification, basic principle, theory of chromatography, TLC, principle and applications.

**Gas Chromatography and HPLC:** Introduction, principle, instrumentation and applications.

**UV-Vis spectroscopy:** Principle. Beer's law, Deviation of Beers law, Instrumentation and applications.

**IR Spectroscopy:** Principle. Fingerprint region, Instrumentation and functional group analysis.

**<sup>1</sup>H NMR Spectroscopy :** Introduction to NMR, quantum description of NMR, chemical shift, spin-spin coupling, coupling constant, instrumentation, applications, interpretation and limitations.

**Mass spectroscopy:** Principle. Fragmentation, Instrumentation and applications.

**Spectroscopic applications:** UV-visible, IR, <sup>1</sup>H NMR, <sup>13</sup>C NMR, mass spectroscopy in structural elucidation of organic compounds. Problems on structural elucidation involving all the above spectroscopic methods.

**UNIT- 2 : Physical Chemistry**

12 hrs

Methods of determining rate laws, collision theory of reaction rates, steric factor, activated complex theory, Arrhenius equation and the activated complex theory, ionic reactions, Kinetic salt effects and steady state kinetics. Kinetic and thermodynamic control of reactions, treatment of unimolecular reactions. Spontaneous reactions, standard free energies change. The law of mass action, Reaction potential, Homogeneous equilibrium, temperature dependence of the equilibrium constant. The hydrodimerisation of acetonitrile, other commercial electro synthetic process, indirect electro synthesis, and the future electro synthesis. Electrochemical sensors. Synthesis of carbon nanotubes and its applications.

**UNIT- 3 : Organic chemistry**

12 hrs

**Aromatic nitro compounds;** Mechanism of nitration, nitro compounds, charge transfer complexes, aromatic nitroso compounds, reduction products of nitro compounds.

**Aromatic amino compounds:** Strength of bases, Hofmann- Martius rearrangement, fischer-Hepp rearrangement, Orton rearrangement, Ullmann reaction and diamines.

**Diazonium salts:** Diazotization, reactions of diazonium salts, diazoamino and aminoazo compounds. Azoxybenzene, azobenzene, hydrozobenzene, benzhidine rearrangement.

**Reactions and rearrangement:** Arndt- Eistert reaction, Baeyer- Villiger rearrangement, Mannich reaction, Oppenauer oxidation, Reformatsky reaction, Sommelet reaction, Stobbe condensation, Witting reaction, Wolf rearrangement, Michael reaction.



**Heterocyclic compounds:** Synthesis and reactivity of furan, thiophene pyrrole, benzofuran, indole, benzothiophene, imidazole, pyrazoles, isoxazoles oxazoles, thiazoles, quinoline, isoquinoline and pyrimidine.

**UNIT-4: Inorganic chemistry**

**12 hrs**

**Co-ordination chemistry :** Introduction of co-ordination compounds, Structural elucidation of coordination compounds by UV- visible, magnetic susceptibility, IR, <sup>1</sup>H NMR and TGA methods.

**Industrial applications of Organometallic compounds:** Homogeneous catalysis, hydrogenations of olefins, oxo-process, Wacker process, water gas shift reactions, carbonization. Heterogeneous catalysis, Fischer- Tropics reaction, Ziegler-Natta polymerization.

**Metal complexes in medicine:** Interaction of metal complexes with nucleic acids, metal ion deficiency effects, toxicity of metal ions and treatment of toxicity, chelating agents in medicine, bacterial agents, antiviral agents and anticancer agents, metal complexes as drugs and therapeutic agents.

**Reference books:**

1. Vogel's Quantitative Inorganic analysis, 7<sup>th</sup> Ed., 2012
  2. G.D. Christian, Analytical Chemistry, 7<sup>th</sup> Ed., Wiley , 2013
  3. Douglas A Skoog, Donald M West, F James Holler and Stanley R Crouch, Fundamentals of Analytical Chemistry, 9<sup>th</sup> Ed, Brooks/Cole, 2014.
  4. Physical Chemistry, 5<sup>th</sup> Ed., - Atkins (ELBS) 1995.
  5. Physical Chemistry - G. M. Barrow (McGraw Hill, Int. St. Ed) 1988.
  6. Fundamentals of Physical Chemistry - Maron and Lando (Collier Macmillan) 1974.
  7. Chemical Kinetics - K.J.Laidler (Harper and Row) 1987.
  8. Principles and Applications of Electrochemistry-Crow (Chapman hall, London) 1988
  9. Advanced organic chemistry – Reaction mechanism & structure – Jerry March.
  10. Reaction mechanism in organic chemistry – S.M Mukharji & S.P Singh
  11. Text book of organic Chemistry – I.L Finar, Vol- I & Vol-2.
  12. Text book of organic Chemistry – R.T Morrison & R.N Boyd.
  13. Reactive intermediates in organic chemistry – N.S Isaacs
  14. Named reaction in organic chemistry – Gurudeep Chatwal
  15. Basic Inorganic Chemistry – 3<sup>rd</sup> edition, F.A Cotton, G.Wilkinson and P.L.Gaw, John Wiley and sons (2002).
  16. Inorganic chemistry – James E Huheey, Harper and Row Publishers (2004)
  17. Inorganic Chemistry – 2<sup>nd</sup> edition, D.F Shriver, P.W. Atkins and C.H. Langford Oxford University Press (1994).
  18. Concise Inorganic Chemistry – J.D. Lee, ELBS
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**Course-IV : CHE SP-IN-4**  
**Field of Specialization-Inorganic Chemistry and Nanoscience**

**Unit-I: Metal complexes:**

**12hrs**

**Synthesis** of Metal Complexes, alkyl and aryl complexes, MOT, CFT: Characterization by UV, IR, NMR and Mass spectrometry .

**Unit-II: Bioinorganic chemistry**

**12hrs**

Essential and trace metals. Metalloproteins as enzymes, vitamin B12, synthetic model compounds,

**Unit-III: Nanomaterials**

**12hrs**

**Synthesis :** Reduction, Sol- gel method, Reverse micelles, combustion method, microwave and co-precipitation method.

**Characterization:** Powder X-ray diffraction (PXRD), Scanning Probe Microscopy (SEM), Transmission electron microscopy(TEM), Atomic force microscopy(AFM)

**Unit-IV: Properties and Application of nanomaterials**

**12hrs**

**Properties of Nanomaterials:** role of size in nanomaterials, Electronic Properties:, Dielectric Properties, Magnetic Properties: Diamagnetic, Paramagnetic, Ferromagnetic and Antiferromagnetic, Optical Properties, Semiconductor nanoparticles, Luminescence in Semiconductor nanoparticles: Photoluminescence, Cathodoluminescence and Thermoluminescence.

**Applications:** Automobiles, Textiles, Cosmetics, Domestic Appliances, Biotechnology and Medical field, Space and Defence, Nanotechnology and Environment

**Reference Books:**

1. Basic Inorganic Chemistry – 3<sup>rd</sup> edition, F.A Cotton, G.Wilkinson and P.L.Gaw, John wiley and sons (2002).
2. Inorganic chemistry – James E Huheey, Harper and Row Publishers (2004)
3. Inorganic Chemistry – 2<sup>nd</sup> edition, D.F Shriver, P.W.Atkins and C.H.Langtore Oxford University Press (1994).
4. Concise Inorganic Chemistry – J.D. Lee, ELBS
5. Organometallic Chemistry – R.C. Mehrotra and A. Singh, 2<sup>nd</sup> Edn., New Age, International Publications, 2006.
6. Bioinorganic Chemistry – A.K. Das, Books & Allied (P) Ltd., 2007.
7. B S Murty, P Shankar, Baldev Rai, BB Rath and James Murday, Textbook of Nanoscience and Nanotechnology, Univ. Press, 2012.
8. Jonathan W. Steed, David R. Turner, Karl J. Wallace, Core Concepts in Supramolecular Chemistry and Nanochemistry, John Wiley & Sons, 2007.

**Course-IV : CHE SP-PC-4**  
**Field of Specialization –Physical Chemistry**

48 hrs

**Unit-I: Introduction to Thermodynamics**

The first and second laws of thermodynamics. Thermodynamic functions, heat capacity, enthalpy, entropy. Equilibrium in one phase system, real gasses, the reactions between gases, reactions of solid-state phases, reaction kinetics, rate equations.

**Theory of Solution and related topics**

The theory of solutions, Free energy as a function of composition. Methods for calculation of thermodynamic equilibrium. Electrochemical processes.

12 hrs

**Unit-II: Polymer Chemistry and Technology**

Monomers, repeat units, degree of polymerization. Linear, branched and network polymers. Classification of polymers. Polymerization: Condensation, addition, radical chain-ionic and co-ordination and co-polymerization. Polymerization conditions and polymer reactions. Polymerization in homogenous and heterogeneous systems, Polymerization Techniques. Number, weight and viscosity average molecular weights. Polydispersity and molecular weight distribution. The practical significance molecular weight. Measurement of molecular weights. End-group, viscosity, light scattering, osmotic and ultracentrifugation methods. Analysis and testing of polymers-chemical analysis of polymers, spectroscopic methods, X-ray diffraction study. Microscopy. Thermal analysis and physical testing-tensile strength. Fatigue, impact. Tear resistance. Hardness and abrasion resistance. Electropolymerization, Drug delivery systems.

12 hrs

**Unit – III Electrochemistry and applications (Related to Research Guide)**

Introduction of electrochemistry, reversible and irreversible cells, Nernt's theory of electrode potential, standard electrode potential, measurement of electrode potential, rate of electrode processes, concentration cells, liquid-liquid junction potential or diffusion potential, applications of EMF measurements, oxidation and reduction systems, Electromotive series or potential series, decomposition voltage or decomposition potential, over voltage, potentiometric titrations, polarography, cyclic voltammetry, theory, instrumentation and applications, solvent effects, supporting electrolytes, reference electrode, working electrode, auxillary electrode, modified electrodes, differential pulse voltammetry, square wave voltammetry, stripping voltammetry, coulometry, amperometric titrations, Introduction, fundamentals of batteries, classification of batteries, sizes of batteries, battery characteristics, primary batteries, dry cell, alkaline  $\text{MnO}_2$  batteries and other batteries. Secondary batteries - lead-acid, alkaline storage batteries-battery

charging theory and practice. Energy economics. Fuel cells - types - electrochemistry of fuel cells. 12 hrs

#### **Unit IV: Quantum Chemistry**

Brief review of Quantum chemistry, Schrodinger equation- Application to one and three dimensional box. Surface chemistry, Theories of adsorption. 12 hrs

#### **Reference books:**

1. Text book of Polymer Science (3<sup>rd</sup> edition) F.W.Billmayer, A Wiley-Interscience, 1984
2. Contemporary Polymer Chemistry (2<sup>nd</sup> edition), H.R.Allcock and F.W.Lampe, Prentice Hall, Englewood Cliffs, New Jersey 1981
3. Polymer Science, V.R.Gowswamy, N.V.Viswanathan and Jayadev Sreedhar, New Age International (P) Limited, August 1996.
4. Physical Chemistry, 5<sup>th</sup> Ed., - Atkins (ELBS) 1995.
5. Physical Chemistry - G. M. Barrow (McGraw Hill, Int. St. Ed) 1988.
6. Thermodynamics for Chemists - S. Glasstone (East-west) 1973.
7. Chemical Kinetics - K.J.Laidler (Harper and Row) 1987.
8. Electrochemistry - Glasstone, Affiliated to East-West Press, 1942.
9. Principles and Applications of Electrochemistry-Crow (Chapman hall, London) 1988.

## Course –IV- CHE SP-OC-4

### Field of Specialization- Organic Chemistry

48 Hrs

[3Hrs/Week]

#### UNIT-I

12 Hrs

##### A. Separation and Purification Techniques:

Principle of: Recrystallization : using various solvents and mixture of solvents :  
Fractional crystallization: e.g. Separation of naphthalene and diphenyl: Fractional distillation : e.g. Separation of Benzene, acetone, ethyl alcohol etc.: Steam distillation: Soxhlet Extraction.

##### B. Biological and Pharmacological Screening of compounds

Principle, material and methodology for the following activities: Antimicrobial (Antibacterial, antifungal and antiviral); Analgesic ; Anti-inflammatory; Anthelmintic and Mechanism of action

#### UNIT-II

12 Hrs

##### A. Oxidations and Reductions in Organic Synthesis

Oxidation reactions involving – Chromium and manganese compounds, air, ozone, hydrogen peroxide, per acids, periodic acid, N-Bromo succinimide  
Reduction reactions involving- Catalytic hydrogenation, Complex metal hydrides, dissolving metals.

##### B. Reagents in Organic Synthesis

- |  |                                    |
|--|------------------------------------|
| 1. Gilman reagent  | 2. Lithium diisopropyl amide (LDA) |
| 3. Dicyclohexyl carbodiimide (DCC)<br>( Reactivity umpolung) | 4. 1,3-Dithiane                    |
| 5. Trimethyl silyl iodide                                    | 6. Tri-n-butyl hydride (TNBH)      |
| 7. DDQ   | 8. Woodward-Prevost hydroxylation  |
| 9. Osmium tetroxide  | 10. Stannic chloride               |
| 11. Selenium dioxide   | 12. Phase transfer catalyst        |
| 13. Crown ether  | 14. Merrifield resin               |
| 15. Bakers yeast   | 16. Peterson synthesis             |

#### UNIT-III : Heterocyclic compounds

12 hrs

Bio significant heterocyclic molecules (Pyrimidine, Pyridine, indole and Purine).  
Synthetic heterocycles as chemotherapeutic agents. (Related to indoles and benzofurans).

Heterocyclic agrochemicals. Naturally accruing heterocycles of physiological importance. Biosynthesis of typical nitrogen and oxygen heterocycles. Recent developments in the chemistry of indoles, benzofurans and benzothiophenes and their comparative study.

**UNIT-IV : Stereochemistry**

**12 hrs**

Topocity and prochirality, Asymmetric synthesis and asymmetric induction, double diastereo selection and double asymmetric induction, diastereo selection in cyclic systems, enantio selective alkylation of ketobne via hydrozones.

**Reference books:**

1. Jaroslava varc-Gajic, Biological Activity of Natural Products (Biochemistry Research Trends) , Nova Science Publishers, 2013.
2. Comprehensive practical organic chemistry-quantitative analysis-V.K.Ahluwalia and university press-Hyderabad.
3. Advanced practical organic chemistry – N.K.Vishnu, second revised edition, Vikas Publication (2000).
4. Quantative & qualitative organic analysis, A.I.Vogel (CBS Publishers, New Delhi-2002).
5. Advanced organic chemistry – Reaction mechanism & structure – Jerry March.
6. Reaction mechanism in organic chemistry – S.M Mukharji & S.P Singh
7. A guide book to mechanism in organic Chemistry – Petersexes
8. Stereo chemistry of carbon compounds – E.L Eliel
9. Stereo Chemistry of carbon compounds – D. Nasipuri
10. Heterocyclic Chemistry- J.Joule and Smith

## Course –IV- CHE SP-CC-4

### Field of Specialization- Inorganic Chemistry

48 hrs

#### CHEMISTRY OF COORDINATION COMPOUNDS

3hrs/week

##### Unit - I: Properties of Coordination Compounds.

12hrs

Objective, nomenclature of metal complexes, EAN.

Spectral properties:-

Types of electronic spectra, selection rules for electronic transitions, charge transfer spectra, d-d transition spectra, energy levels in tetrahedral field, Tanabe-Sugano diagrams.

Magnetic properties of the Complexes:

Origine of magnetic moment, magnetic permability and susceptibility, diamagnetism, paramagnetism, ferromagnetism and anti ferromagnetism.

##### Unit-II: Theories of Coordinate Bond

12hrs

The Valence Bond Theory; modification of Paulings VBT, drawbacks of VBT,

Crystal Field Theory (CFT); Splitting of d-orbitals in octahedral field, CFSE for tetrahedral symmetry, tetrahedral distortion in octahedral symmetry, square planar coordination, orbital splitting in other fields, adoption of geometrical arrangements, magnitude of  $10Dq$ , evidence for CFSE in complexes.

The crystal field model. Molecular Orbital theory: MOT for sigma bonding in complexes, MOT and other geometries,  $\pi(\pi)$  bonding and MOT. Adjusted Crystal Field Theory. A review of theories.

##### Unit-III : Thermodynamic Stability of the Metal Complexes:

12hrs

Kinetics and thermodynamic stability of the metal complexes, factors affecting the metal complexes, chelate and macro cycle effects, structural equilibria of complexes and mixed ligand complexes. Calculation of  $\Delta G^\circ$  and  $\Delta H^\circ$ , factors influencing the stability of complexes, correlation between the properties of ligand and stability of metal complexes, Determination of stability by spectrophotometric- Job's, mole-ratio, slope ratio,  $p^H$  metric (potentiometric), polarigraphic, solvent-extraction and ion-exchange method.

##### Unit-IV: Isomerism of Metal Complexes

12hrs

Isomerism of Metal Complexes:

Ionization isomerism, solvent isomerism, linkage isomerism, coordination isomerism, ligand isomerism, polymerization isomerism.

Stereoisomerism: cis-trans isomerism, optical isomerism.

Identification of isomeric metal complexes: By conductivity measurement, by electrolysis, by freezing point depression, by IR, by XRD, by Dipolement, by NMR spectroscopy, by mass spectroscopy and by Chemical method.

**REFERENCES:**

1. Chemistry (Volume-II), Inorganic Chemistry, Shyam Singh, Himalaya Publishing House, First Edition-2010.
2. Theoretical Principles of Inorganic Chemistry, G.S.Manku, Tata McGraw Hill Publishing Company Limited, New Delhi, Sixteenth reprint-2012.
3. Text Book of Inorganic Chemistry, R.Gopalan, Univeristies Press, Hyderabad-2012.
4. Concise Coordination Chemistry, R.Gopalan and V.Ramalingam, Vikas Publishing House Pvt.Ltd., New Delhi, Reprint-2012.
5. Advanced Inorganic Chemistry, O.P.Agarwal, Dhanpat Rai and Sons, New Delhi, Eighth Edition-2012.
6. Chemistry of Complex, Equilibria, M.T.Beck, Rinhold, London-1990.
7. Inorganic Chemistry, J.E.Huheey, E.A.Keiter and R.L.Keiter, 4<sup>th</sup> Edition-1993.
8. Magneto Chemistry, R.L.Carlin, Springer Verlag.
9. Balic Inorganic Chemistry, F.A.Cotton, G.Wilkinson and P.L.Gau, Jhon Wiley and Sons, Inc., Edition-1999.



## Course –IV- CHE SP-OM--4

### Field of Specialization: Organometallic Chemistry

**48 hrs, 3 hrs/week**

#### Unit-I

A Brief history of Organometallic Chemistry, ligands, types of ligands, ligands derived from  $4n\pi$  electron system. Methods of synthesis of organometallic compounds. Techniques of handling air and moisture sensitive organometallic compounds. Ferrocene, bis- Iron fulvalene and their properties.. MOT representations of ferrocene. 12hrs

#### Unit-II

Electronic interactions in Organometallic compounds. Robin and Day classification, class II-III compounds. Hush Theory. Methods for probing the electronic interactions, cyclic voltammetry, UV-Visible, FTIR and Mössbauer spectroscopy. Spectroscopic time scales. Introduction to theoretical chemistry. –*Ab-initio* methods, Basis sets and calculations 12hrs

#### Unit-III

Synthesis of pentalene, indacene, dicyclopenta dienyl naphthalene, tris pyrazoloyl borate ligands and their methylated derivatives. Poly ferrocenes, pyrazoloyl borate –acetylene complexes, synthesis and applications. 12hrs

#### Unit-IV

Synthesis of organometallic cluster compounds. Building block approach with special reference to acetylene bridged metal compounds. Study of zero field splitting, quantum magnetic tunnelling and spin-spin interaction. Magnetic properties of organometallic clusters and experimental measurements of magnetic properties. Magnetic property measurements- principles and methods. 12hrs

#### References:

- 1) Organometallic chemistry, a unified approach, R C Mehrotra, A. Sing. New age international publishers and the references there in.
- 2) Robin, M.B.; Day, P. Advanced inorganic chemistry and radio Chemistry, 1967, 10, 247-422.
- 3) Kealy, T.J ; Pauson P.L, Nature 1951, 168, 1039-1040.
- 4) Barlow, S; Murphy, V. J.; Evans, J.S.O.; O'Hare, D. Organometallics, 1995, 14, 3461-3474
- 5) N.S.Hush, Progr.Inorg.Chem.8,391 (1967).
- 6) Sinha, U.; Lowery, M. D.; Hammack, W. S.; Hendrickson, D. N. Drickamer, H. G. J. Am. Chem. Soc. 1987, 109, 7340-7345
- 7) Sengupta S.C; Bhattachargee, A. Jour.Indian Chem.Soc, 1953, 30(12) 805-808
- 8) Stephen Barlow and Dermont O hare Chem.Rev 1997 vol 97, No 3.
- 9) I. Levine: Quantum Chemistry: Allyn and Barrown .Inc. Boston(1970)

10) R.G Parr, W. Yang, Density functional theory of atoms and molecules. Oxford University Press, New York (1971)

11) P. Gülich, E. Bill, A. X. Trautwein *Mössbauer Spectroscopy and Transition Metal Chemistry*  
Springer, 2011