KARNATAK UNIVERSITY, DHARWAD

DEPARTMENT OF STUDIES IN CHEMISTRY

Ph.D. Course work

Course I: Research Methodology (Common to all)

Total: 48 hrs

1. **Nature and Scope of research in Chemistry:** survey of literature (use of computer devices in literature survey, location of journals). Need of literature survey. Research areas, Theatrical and fundamental research, Inter disciplinary research.

   8 hrs

2. **Research problem:** literature survey, choice of research problem, writing research papers/review article research proposal/ dissertation/ Synopsis, Thesis, Research journals in chemistry, significance of research publications in terms of impact factors, H-index etc, conferences, work-shops. Conventions (their organizations).

   10hrs

3. **Intellectual Property Rights:** intellectual property rights: Concept and evolution. Law of designs. Law of copy rights and trademarks. Law of patents.

   6hrs

4. **Application of Computers in Chemistry:** Software's used in chemical research (Chemdraw ultra, Chemsketch). Internet for Chemists: Online Search of chemical data bases and online journals. Search engines in chemical research viz. Sci-finder, Scopus, Beilstein cross fire etc.

   8hrs

5. **Recent advances in Chemistry:** Outstanding discoveries and Novel prizes in Chemistry during last five years.

   7hrs

6. **Statistical treatment of analytical data:** Reliability of results-confidence interval. Estimation of detection of limits. Significant numbers. Comparison of results-Student's test, comparing the two means and standard deviation F-test, t-test and paired t-test and paired t-test. Rejection of a result: Q-test. Number of replication determination. Correlation and regression-correlation coefficient, linear regression.

   9hrs

KARNATAK UNIVERSITY, DHARWAD

DEPARTMENT OF STUDIES IN CHEMISTRY

Ph.D. Course work

Course II: Cognate/Core subject: Chemistry (Common to all)

Total: 48hrs

1. **Separation techniques:** Chromatography in chemical research, Principle, theory application of thin layer chromatography, gas chromatography (GSC and GLC), HPLC application of GCMS.

   8hrs

2. **Instrumental methods in chemical research:** Introduction, theory, instrumentation application of the following in the structural elucidation of organic compounds as well as in complexes.

   i. IR/FTIR spectroscopy.
   ii. UV/Visible spectroscopy.
   iii. ^{1}H and ^{13}C NMR, ESR spectroscopy.
   iv. Mossbauer spectroscopy and X-ray diffraction studies.

   22hrs

3. **Thermal analysis:** Introduction, theory, instrumentation and applications of TGA, DTA and DSC.

   5hrs

4. **Green Chemistry:** Biocycles, green chemistry in day today life, principles, synthetic methods, industrial applications.

   7hrs

5. **Nanomaterials:** Introduction to ‘nanomaterials, physical and chemical properties of nanomaterials, applications of nano technology.

   6hrs

KARNATAK UNIVERSITY, DHARWAD

P.G. DEPARTMENT OF STUDIES IN CHEMISTRY

Course-work for Ph.D

PAPER –III(OPTIONAL)

Advanced coordination chemistry (Inorganic)

1.Ligand Systems:

Novel ligand systems containing O,N, S, P as coordinating sites, cyclic and acyclic ligand systems, ligands with high denticity.

4hrs

2.Preparations of coordination compounds:

Preparative methods : Simple addition reactions, substitution reactions, oxidation-reductions, Thermal dissociation methods, Preparations in inert atmosphere, Reactions of coordinated ligands, Preparations involving trans and cis effects, other methods of preparing coordination compounds.

6hrs

3. Theories of transition metal compounds:

Crystal field theory: Crystal field splitting in weak field, strong field and intermediate field. Non- octahedral complexes, Tetrahedral complexes, square planar complexes, other stereo chemistries.

Molecular orbital theory: Introduction, Octahedral complexes, metal-ligand σ interactions,metal ligand π interactions. Tetrahedral complexes and complexes with other geometries.

8hrs

4. Electronic spectra of transition metal complexes:

Term symbols for d^n ions, spectroscopic ground states, selection rules.Spectral bands-band shapes, band width, band intensities. Effect of spin-orbit coupling, Orgel diagrams, Tanabe-Sugano diagrams, Racah parameters, Interpretation of spectra of octahedral, tetrahedral, square planar and other geometries. Charge transfer spectra,Intervalence charge transfer.

7hrs

5. Magnetic properties of transition metal complexes:

Introduction, classical magnetism, orbital contribution,orbital contribution reduction factor, spin-orbit coupling, diamagnetic corrections, magnetically non-dilute compounds.Spin equilibria.

5hrs

6. f- electron system:Lanthanides and actinides:

Electronic structure of the Lanthanide and actinide ions,spin-orbit coupling. Excited state of f –electron system.Electronic spectra of f- electron system, Crystal field and f-f intermediates.f-d and charge transfer transitions. Magnetism of Lanthanide and actinide ions

5hrs

7. Other methods of studying coordination compounds:

Vibrational spectroscopy, Resonance Raman spectroscopy, spectroscopic methods unique to optically active molecules.

NMR and Mossbauer Spectroscopy. Electron paramagnetic resonance spectroscopy.Photo electron spectroscopy. Fluorescence.Molar Conductivities, Cyclic VoltammetryX-ray crystallography.

15hrs

8. Reaction mechanism in transition metal complexes:

Energy profile of a reaction, inert and labile complexes, kinetics of octahedral substation and mechanistic aspects. Acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism and evidences in its favour. Anation reactions, Substitution reactions in square planar complexes, trans effect, mechanism of substitution. Electron transfer reactions- inner sphere and outer sphere reactions, complimentary and Non-complimentary reactions.

Photochemistry of metal complexes- types of photochemical reactions, photo substitution and photo redox reactions and solar energy conversions.

10hrs

References:

1. Physical Inorganic Chemistry, S. F.A.Kettle. Spectrum Publisher(1995).

2. Comprhensive CoordinationChemistry,Eideted By G.Wilkson and Others Vol.1-7. Pergamon Press (1987).
3. Physical Methods in Inorganic Chemistry, R.S. Drago.SaunderCollege.(1996).
4. Fundamentals of Molicular Spectroscopy C.N.Banwell. Ind.E.M.McCash,Tata McGraw-Hill Ltd(2001)
5. Structural Meathods in Inorganic Chemistry E.A.EbsworthD.W.H.Ranbin and S.Cradock, ELBS(1987).
6. Infrared Spectra of Inorganic and coordination compounds, K.Nakamoto. Wiley Interscience(1986).
7. Intoduction to Spectroscopy, Pavia, Lampman and Kriz .,Thomson Learning(2001).
8. Electronic Absorption Spectroscopy and Related Techniques ,D.N.Satyanarayana ,OUP,(2001).
9. Inorganic Reaction Mechanism- F.Basoloand R.G.Pearson, Wiley Eastern, (1979).
10. W.W Porter Field : Inorganic Chemistry – A Unified Approach, Elsevier, (2005).

KARNATAK UNIVERSITY, DHARWAD
DEPARTMENT OF STUDIES IN CHEMISTRY
Ph.D Course Work
Course III: Advanced Organic Synthesis (Organic) Optional

Total : 48Hrs

1. Synthesis of Sydnones, Coumarins, Chromones, Benzimidazoles, Indoles, Quinolines, thiazoles, Fused thiazoles, Oxadiazoles, thiadiazoles, imidazothidiazoles and their reactions (thermal, photochemical and rearrangements), oleochemicals and their applications

2. Heterocycles in biological systems and drugs: Imidazoles, NADH, Isoalloxazines, Pyridoxal, pteridines, folic acid, Vit - B_{12} and their role in biological systems. Fatty acid metabolism and their biosynthesis.

3. Synthesis and mechanism of action of sulphapyridine, sulphathiazole, sulphamerazine, sulphamethazine, cephalosporins, ciprofloxacin, enosacin, nalidixic acid, rifampicin.

4. Newer reactions and reagents:

Newer reactions: Des - martin oxidation, Buchwald - Hartwig, Sonogashira and Stille cross Coupling reactions, Corey - Bakshi - Shibata reduction, Dimroth rearrangement, Heck arylation, Sharpless aminohydroxylation and dihydroxylation.

Newer reagents: NBS, DCC, Fermy's salt, LDA, DDQ, Wilkinson catalyst, Gillmann reagent.

5. Retrosynthetic analysis of functionalised aliphatic, aromatic and simple heterocyclic compounds involving single and multiple C-C and C-X disconnections. Concept of synthons, Synthetic equivalents, FGI, Functional group interconersions of aromatic and mono and biheterocyclic compounds involving oxidation, reduction, substitution, addition, elimination and rearrangement reactions.

6. Carbon - Carbon forming reactions: Applicaton of acid, base and metal catalysed reactions of functionalized organic compounds involved in multistep synthesis.

REFERENCE BOOKS AND WEBSITES:

1. Modern Synthetic Reactions by H.O.House, W.A. Benzamin, INC, London(1972).
2. Biochemistry by D.E.Metzler, Academic Press, New York (1977).
3. Principles of Organic Synthesis by R.O.C. Norman, J.M.Coxon. 3rd Edition (2001), Nelson Thornes Cheltenham UK.
4. Organic Chemistry vol - I & II by I.L.Finar, Orient Longman (indian edition), 2005.
5. Organic chemistry by F.A.Carey 4th edition. McGraw Hill 2000 New York.
6. Heterocyclic chemistry by M.M. Jovles and smith 5th Edition, Viley, 2010.
7. Strategic applications of named reactions in organic synthesis by Barbara Czako and Laszlo Kurti, Elsevier, 2005.
8. Modern methods of Organic synthesis by Carruthers.
9. Disconnection approach, Stuart Warren.

KARNATAK UNIVERSITY, DHARWAD

DEPARTMENT OF STUDIES IN CHEMISTRY

Ph.D. Course work

Course III: Advanced Polymer Chemistry (Physical) Optional

Total 48hrs

1. **Analytical Methods:** Types of errors. Mean value and standard deviation, standard deviation and probability. Methods of least squares. Calibration curves. Significant figures, significant figures in arithmetic, significant figure and graphs.

   9hrs

2. **Characterization and analysis of polymer surface:** Gel permeation chromatography (GPC), scanning electron microscopy (SEM), transmission electron microscopy (TEM), electron spectroscopy for chemical analysis (ESCA), atomic force microscopy (AFM), photo-acoustic spectroscopy (PAS) and attenuated total reflectance spectroscopy (ATR).

   10hrs

3. **Pervaporation:** An overview, history, definition, theory, sorption in membranes, diffusion in membranes, performance parameters, influence parameters, advantages and disadvantages, applications. Types of membranes, membrane modules, tubular modules, hollow fiber modules, plate and frame systems, spiral wound modules.

   10hrs

4. **Nonlinear optical materials:** Definition and history. Basic aspects of nonlinear optical phenomena, reaction between molecular and macroscopic properties, linear optical effects, nonlinear optical effects, second harmonic generation (SHG). Experimental methods: Kurtz-Perry powder technique, electric field induced second harmonic generation, Hyper-Rayleigh scattering, Maker fringe technique. Electric field poling methods, relaxation of SHG in poled polymers. Basic molecular characteristics of nonlinear optical (NLO) materials, second-order NLO materials, application of NLO materials.

   10hrs

5. **Drug delivery systems:** Concepts and system design, fundamental of rate-controlled drug delivery, oral/targated drug delivery systems, micro- and nano-particles transdermal systems, nasal and occulary systems, protein and gene delivery systems, patient compliance, in-vitro and in-vivo testing of drug delivery system, drug-conjugates, micro-encapsulation.

   9hrs

REFERENCES

1. D. C. Harris, Quantitative Chemical Analysis, 5th Edition, W. H. Freeman and Company, New York, 1998.

2. D. A. Skoog, D. M. West, F. J. Holler, Analytical Chemistry, Harscourt Brace College Publishers, Landon 1994.

KARNATAK UNIVERSITY, DHARWAD

DEPARTMENT OF STUDIES IN CHEMISTRY

Ph.D. Course work

Paper III: Polymer Blends

Total: 60 hrs

1. **Concepts and Definitions:** Polymer, Monomer, Oligomer, Repeating Unit, Degree of Polymerization and Functionality. Copolymers-Random Copolymer. Alternating Copolymer, Graft Copolymer, Block Copolymer, Addition and Condensation, Organic and Inorganic, Homopolymer and Copolymers, Linear, Branched and Cross-linked Polymers. Thermoplastics and thermosets, Elastomers and fibres.

12hrs

2. **Thermoplastics Materials and Rubber:** Introduction to thermoplastic and plasticisers-Poly (ethylene glycol) and Glycerol.**Thermoplastic Materials**- Vinyl Plastics-Ploy(ethylene), Poly (vinyl chloride), Poly (vinyl acetate), Poly (ethylene vinyl acetate), Poly(propylene), Poly(styrene), Poly (vinyl alcohol), Poly (vinyl pyrrolidone), Fluorocarbon Thermoplastic: poly(tetrafluoroethylene). Cellulose Base Plastics – Cellulose acetate, Cellulose acetate butyrate, Cellulose acetate propionate, Polyamide-Nylon 6,6. **High Temperature Thermoplastics**: Poly(imides), Poly(sulphones), Poly (ether ether ketone). **Elastomers;** Natural Rubber, Vulcanization, Styrene-Butadiene Rubber, Butadiene Rubber, Butyl Rubber, Silicone Rubber.

12hrs

3. **Thermosets:** Introduction. **Thermoset Materials:** Phenolics-Phenol Formaldehyde, Urea Formaldehyde, Melamine Formaldehyde**. Polyester resins** – Polyesters, Alkyd Resins. Polyurethanes, Epoxy Resins, Polyimides, Silicones.

12hrs

4. **Preparation of Polymer Blends:** Definition of Polymer Blend. Advantage and Reasons of Blending, Polymers Blending technique's-melt Blending (Mixing), Latex Blending, Solution Blending.
   Types of Polymer Blends- Miscible Polymer Blend and immiscible Polymer Blend. Basic Thermodynamics. Blend Morphology.

12hrs

5. **Characterization Technique: Techniques:Thermal Analysis Techniques**-Differential Scanning Calorimetry (DSC), Thermogravimetry Analysis (TGA), Microscopy Techniques- Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM) and Atomic Force Microscopy (AFM), Mechanical Behaviour-Universal Testing Machine (UTM), Amorphous and Crystallinity-XRD, Spectroscopy Technique-FT-IR.

12hrs

KARNATAK UNIVERSITY, DHARWAD

DEPARTMENT OF STUDIES IN CHEMISTRY

Ph.D. Course work

Paper-III (Optional)

Advanced Analytical Chemistry

1.Statistical Analysis: Evaluating the Data

Evaluation of analytical data, precision and accuracy, normal distribution curve, graphical presentation of results, method of average, method of linear least square, statistical aid to hypothesis, t–test, F-test, chi-square test, rejection of data. Use of Excel sheets in the treatment of analytical data.

5hrs

2. Electroanalytical techniques:

Voltammetry: General Introduction, principle, instrumentation and applications of cyclic voltammetry, differential pulse voltammetry, square wave voltammetry and stripping voltammetry with special emphasis on the assay of bioactive compounds/drugs and/or their interactions with biomolecules (proteins and DNA).

Electrochemical sensors: Modified electrodes, types of modified electrodes, their fabrication, modified electrodes (with C_{60}, CNTs, graphene, metal oxide nano particles) as voltammetric sensors and biosensors for analytical and binding applications.

10hrs

3.Spectral methods of analysis

i) Spectroflourometry:Construction of Jablonski diagram, photophysical pathways of excited molecular system (radiative and non-radiative), phosphorescence, fluorescence quenching: quenching by excimer and exciplex emission, factors affecting quenching, Stern-Volmer and modified Stern-Volmer equation, Fluorescence resonance energy transfer between donor (protein) and acceptor (quencher) molecules. Types of quenching mechanisms and analytical applications of quenching with special emphasis on drug-protein and drug-DNA interactions,

and assay of drugs. Evaluation of binding and thermodynamic characteristics of interactions.Applications of fluorescence life time, synchronous and 3-D fluorescence.

14hrs

ii). Ultraviolet and visible spectroscopy: Introduction, laws of absorption, instrumentation, applications with emphasis on assay of drugs (anticancer, antihypertensive, antiallergic and anti-inflammatory). 4hrs

iii). FT-IR: Introduction, sampling technique, absorption of common functional groups, factors affecting IR bands,utility of FTIR in the study of biomolecular interactions.

iv). Circular dichroism: Fundamentals, CD curves and applications in the characterization of ligand-biomolecule interactions.

3hrs

4.**Recent advances in Analytical Chemistry**: Recent papers published in Talanta and Analytical Chemistry Journals during the last two years.

9hrs

References

1.Instrumental Analysis-D. A. Skoog, F. J. Holler and S. R. Crouch, Cengage Learning (2010).

2. Analytical Chemistry-G.D. Christian, 5th ed., John Wiley & Sons, Inc, India (2001).

3. Instrumental methods of analysis,7th Ed.-H.H.Wlliard, L.L.Merrit and J.J. Dean(1988).

4. Fundamental of Analytical Chemistry-D.A. Skoog, D.M. West, Holler and Crouch, 8thedition,Saunders College Publishing, New York (2005).

5. Principles of fluorescence spectroscopy-J. R. Lakowicz, 3rd Edition, Springer publication (2006).

6. Introduction to spectroscopy-D. L. Pavia, G. M. Lapman and G. S. Kriz, 3rdEdition, Thomson (2001).

7. Lehninger Principles of Biochemistry-A. L. Lehninger, M. Cox, D. L. Nelson, W. H. Freeman & Co. Publication (2005)

8. DNA structure and function- R. R. Sinden, Academic Press(2006).

9. www.sciencedirect.com

10. www.acs.org