



**DEPARTMENT OF CHEMISTRY,  
PALAMURU UNIVERSTY, MAHABUBNAGAR, TELANGANA**

**Ph. D. COURSE WORK  
Effective from 2021-2022**

*By*  
2/9/23



DEPARTMENT OF CHEMISTRY  
PALAMURU UNIVERSITY, MAHABUBNAGAR, TELANGANA  
Ph. D. Course Work – Chemistry

Paper – I

RESEARCH METHODOLOGY

Unit-I – Research Methodology

Marks:100

Research Formulation:

Motivation and objective of research problem. Selecting the problem, Necessity of defining the problem – importance of literature review in defining a problem – Literature review – Primary and Secondary sources – reviews treatise and monographs – patents – web as a source – searching the web – critical literature review – Identifying gap areas from literature review - Development of working hypothesis. Research design – Basic Principles – Need of research design – Features of good design – Important concepts relating to research design – Observation and Facts. Laws and Theories. Prediction and explanation. Induction. Deduction. Development of models. Developing a research plan – Exploration. Description. Diagnosis, Experimentation – Methods of data collection – Sampling Methods – Data processing and analysis strategies.

Reporting and thesis writing:

Structure and components of scientific reports - Types of report – Technical reports and thesis-significance – Different steps in the preparation – Layout. Structure and Language of typical reports – Illustrations and tables - Bibliography. Referencing and foot notes – oral presentation – Planning – Preparation – Practice – Making presentation – Use of visual aids – Importance of effective communication – Research Ethics – Reproduction of published material – Plagiarism - and acknowledgement.

Unit – II: Thermal methods and Electron Probe Techniques

Thermal methods of analysis: Thermogravimetry. Differential Thermal analysis and Differential Scanning calorimetry. Instrumentation. Methodology of TG. DTA. and DSC.

Atomic Absorption Spectroscopy (AAS): Principles of AAS. Instrumentation – flame AAS and furnace AAS, resonance line sources (hallow cathode lamp, electrode less discharge lamp), sample introduction system (pneumatic nebulizer), sensitivity and detection limits in AAS, interferences-chemical and spectral, evaluation methods in AAS and applications in qualitative and quantitative analysis.

Electron Probe Techniques: Scanning electron microscopy (SEM) – Principle. Instrumentation, applications, Transmission Electron Microscopy (TEM) – Principle. Instrumentation, applications. Energy Dispersive X-ray spectroscopy (EDX) – Principle. Instrumentation, applications.

Theory and principles of fluorescence spectroscopy. Characteristics of fluorescence emission. Fluorescence life time. Quantum yield, static and dynamic/collisional quenching and comparison. Fluorescence polarization and polarization spectra of fluorophore. Applications of fluorescence quenching.

Brunauer-Emmett-Teller (BET) - Principle, instrumentation, determination of surface area using BET Equation.

A. Padmahi.

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K. Ramesh.

K. S. Jale

P. L. S.

G. S. S.

B. S. S.



### Unit – III: $^1\text{H}$ and $^{13}\text{C}$ NMR Spectroscopy

$^1\text{H}$  and  $^{13}\text{C}$  NMR Spectroscopy: Introduction, Principle, Instrumentation and applications of  $^1\text{H}$  and  $^{13}\text{C}$  NMR Spectroscopy. First order and non-first order spectra eg: AX, AX<sub>2</sub>, AX<sub>3</sub>, A<sub>2</sub>X<sub>3</sub>, AMX, AB and ABC. Nuclear Overhauser Enhancement (NOE).  
Mass spectrometry, GC-MS and LC-MS: principle of mass spectrometry. Instrumentation and Applications of mass spectrometry. Principles of EI, CI, Fast Atom Bombardment (FAB).  
Secondary Ion mass spectrometry (SIMS), Electrospray ionization (ESI), Matrix Assisted Laser Desorption Ionization (MALDI). High Resolution Mass spectrometry (HRMS) Introduction, instrumentation and applications of gas chromatography- Mass spectrometry (GC-MS) and Liquid Chromatography- mass spectrometry (LC-MS) techniques.  
Chromatography: Principle and applications of TLC and Column Chromatography. Principle. Instrumentation and applications of GC and HPLC

### Unit –IV: Vibrational, X-Ray spectroscopy and Diffraction Techniques:

#### Vibrational Spectroscopy:

Infrared spectroscopy – Interaction of electromagnetic radiation with matter. Selection rules. Principle and instrumentation of FTIR.

Raman spectroscopy – Raman effect. Complementary nature of IR and Raman spectra. Typical applications of Raman spectroscopy – Structure, determination of molecules from IR and Raman spectroscopic techniques.

Electronic spectroscopy: Elementary energy levels of molecules – selection rules for electronic spectra: types of electronic transitions in molecules. Chemical analysis by electronic spectroscopy.

#### X-ray Spectroscopy:

X-ray fluorescence (XRF): Experimental method. Processes in X-ray fluorescence. K- emission spectrum of tin. L- emission spectrum of gold.

X-ray absorption: Absorption techniques. Absorption edge fine structure (AEFS spectra) and extended X-ray absorption fine structure (EXAFS) spectra.

**Diffraction Techniques:** X-ray diffraction: experimental methods of X-ray diffraction. Primitive and non-primitive unit cells. Indexing the reflections. Identification of unit cells from systematic absences in diffraction pattern. Structure factor and its relation to intensity and electron density. Description of the procedure for an X-ray structure analysis. Typical examples.

#### References:

1. An introduction to research methodology. Garg.B.L.Karadia. R. Agarwal. F. and Agarwal. U.K. .2002 RBSA publishers.
2. Kothari. C. R. 1990 Research Methodology Methods and Techniques New Age International. 418p.
3. Principles of Instrumental Analysis. Skoog. Holler. Nieman. 5<sup>th</sup> ed., Harcourt College publishers. 1998.
4. Analytical Chemistry- Gary D. Christian. 6<sup>th</sup> ed., John Wiley and sons. Inc. New York 1994.
5. Instrumental methods of Analysis – Willard. Merit. Dean. 6<sup>th</sup> ed. CBS Publishers & distributors. 1986.

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6. Hand Book for Instrumental Techniques for Analytical Chemistry. Ed. Frank Settle. Prentice Hall. New Jersey. USA .1997.5. Vogel's Text book of Quantitative Analysis – GJ Jeffery. J. Basse 5<sup>th</sup> ed. Longmann. ELBS Publications. 2000.
7. Principles and practice of Analytical Chemistry. F. W. Field & D Kealey. 5<sup>th</sup> Ed. Blackwell Science. 2000.
8. Quantitative Chemical Analysis. Danial C. Harris. 6<sup>th</sup> Ed. W H Freeman & Co. New York. 2003. 8. Analytical Chemistry: An Introduction. Crouch. 7<sup>th</sup> Ed. Saunders College Publishing. 2000.
9. Spectroscopic Identification of organic compounds by R.M. Silverstein and F. X. Webster.
10. Organic spectroscopy by William kemp
11. Mass spectroscopy by William kemp
12. Spectroscopic methods in organic Chemistry by D. H. Williams and I Fleming
13. Biological Mass spectrometry by A. L. Burlingame
14. Principles and Practice of Biological Mass Spectrometry by Chhabil Das
15. Spectroscopic identification of organic compounds by R.M. Silversten. G.C Bassler and T.E. Mosrill
16. NMR – A multinuclear introduction by William Kemp
17. Techniques and Properties of Chromatography by Scott Raymond P.W.
18. Principles and Practice of modern Chromatographic methods by K. Robards, P.R. Haddad and Peter E. Jackson
19. Fundamentals of Molecular Spectroscopy. Banwell & McCash
20. Introduction to Molecular Spectroscopy. G.M. Barrow. McGraw Hill
21. Molecular Spectroscopy, J.D. Graybeal. McGraw Hill
22. Basic Principles of Spectroscopy. R Chang. McGraw Hill
23. Physical Methods for Chemistry. R. S. Drago. Affiliated East West Press
24. Vibrational Spectroscopy: Theory and Applications D.N. Sathyanarayana. New Age International
25. Introduction to Raman Spectroscopy. J.R. ferraro & K. Nakamoto. Academic press
26. X –ray diffraction procedures for polycrystalline and amorphous materials. H. P. Klag & L. Alexander. John Wiley
27. Physical Chemistry. N. Levine. McGraw Hill
28. Atkin's Physical Chemistry P. Atkins & Julio de Paular Oxford University Press
29. Molecular structure and Spectroscopy, G. Aruldas. Eastern Economic Edn.

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DEPARTMENT OF CHEMISTRY  
PALAMURU UNIVERSITY, MAHABUBNAGAR, TELANGANA

Syllabus for Ph.D. Course Work  
Paper-II: Inorganic Chemistry Specialization  
(Effective from Academic year)

(Approved in the PG Board of studies held on

)  
Marks:100

**Unit-I: Bonding in Metal Complexes, Electron absorption Spectroscopy**  
**Molecular Orbital Theory of Metal Complexes:** Introduction to Molecular Orbital Theory. Symmetry Classification of Metal and Ligand Group Orbitals in Cubic and Non-Cubic Environments: Octahedral, Tetrahedral, Square Planar, Square Pyramidal, Trigonal Bipyramidal Geometries – Concept of Ligand Group Orbitals – Construction of Molecular Orbital Energy Level Diagrams -Octahedral, Tetrahedral and Square Planar Metal Complexes with sigma( $\sigma$ ) & Pi ( $\pi$ ) Bonding contribution from the Ligands.  
**Electron absorption Spectroscopy:** Effect of weak cubic crystal fields on S, P, D and F terms- Orgel diagrams Selection rules: Relaxation in selection Rules-Nature of Electronic Spectral Bands: Band widths, Band Intensities and Factors influencing Band Shapes –Crystal Field Spectra of Oh and Td Metal Complexes of 3d Metals. Calculation of 10Dq Values, Racah Parameter.

**Unit-II: IR, Raman, X-ray Photoelectron Spectroscopy and ESR**  
**IR and Raman:** Symmetry Based Selection Rules of IR and Raman –Symmetry requirements for overtone, Binary and Ternary Combination bands- Fermi resonance. Application of IR spectroscopy in the structural elucidation of Inorganic compounds and Metal Complexes-Aquo, Sulfato, Carbonato, Nitro and Carbonyl metal complexes.  
**Photoelectron Spectroscopy:** Principle and Instrumentation, Types of Photoelectron Spectroscopy – UPS & XPS. Binding Energies, Koopman's Theorem, Chemical Shifts. Photoelectron Spectra of Simple Molecules: N<sub>2</sub>, O<sub>2</sub>, F<sub>2</sub>, - Vibrational Structure of PES Bands, Potential energy curves, Interpretation of Vibrational spectral data for ionized (M<sup>+</sup>) species, Prediction of Nature of Molecular Orbitals. ESCA in qualitative analysis, Principles of Auger electron spectroscopy.  
**Electron Spin Resonance:** Introduction, principle, instrumentation, selection rules, interpretation of Lande's factor 'g'. Hyperfine and super hyperfine Coupling. Anisotropy in 'g' values and hyperfine coupling constants. Zero field splitting, Kramer's degeneracy and quadrupolar interactions. Study of free radicals and transition metal complexes. Evidence for covalency in complexes, ex. Cu(II) Bis-salicylalimine, Bis-acetylacetonatovanadyl(II) and hexachloroiridium(IV) complexes.

**Unit-III: Nanomaterials**

**Nanoparticles and their applications:** Introduction to nanoparticles. Reduced dimensionality in solids – zero dimensional systems, fullerenes, quantum dots. One dimensional systems, carbon nano tubes, preparation of nano particles –top down and bottom up methods. Preparation of nanomaterials- – sol-gel methods, and chemical vapour deposition method; thermolysis. Characterization of nanoparticles – experimental methods – powder X-ray diffraction, transmission electron microscopy (TEM), and atomic force microscopy (AFM) (detailed theory

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and instrumentation are not required). Optical properties of nanoparticles, Applications of nanoparticles.

#### Unit-IV: Bio-Inorganic Chemistry

**Metal ions in Biological systems:** Brief survey of metal ions in biological systems. Effect of metal ion concentration and its physiological effects. Basic principles in the biological selection of elements. Oxygen transport and storage: Hemoglobin (Hb) and Myoglobin (Mb) primary, secondary, tertiary and quaternary structures and non-covalent bonds present in them. Oxygenation equilibria for Mb and Hb. Factor effecting oxygenation equilibria. Co-operativity and its mechanism. Spin state of iron. Spatial and electronic aspects of dioxygen binding. Allosteric models (T and R states). Role of globin. Transport of NO and CO<sub>2</sub>. Hemocyanin (Hc) and Hemerythrin (Hr): Introduction-structure of active sites with oxygen and without oxygen. Comparison of Hemerythrin and Hemocyanin with hemoglobin. Photosynthesis: Structural aspects of Chlorophyll. Photo system I and Photo system II. Vitamin B6 model systems: Forms of vitamin B6 with structures. Reaction mechanisms of (1) Transamination (2) Decarboxylation and (3) Dealdolation in presence of metal ions.

**Platinum Complexes in Cancer therapy:** Discovery, applications and structure effect relationships. *Cis-platin* (Cis[Pt(NH<sub>3</sub>)<sub>2</sub>Cl<sub>2</sub>] mode of action. Drug resistance and DNA repair mechanism.

#### References:

1. Fundamentals of Molecular Spectroscopy, Banwell and McCash.
2. Introduction to Molecular Spectroscopy, G. M. Barrow.
3. Introduction to Spectroscopy, Pavia Lampman Kriz.
4. Structural methods in Inorganic chemistry, E.A.V. Ebsworth.
5. Advanced Inorganic Chemistry. F.A.Cotton, G.Wilkinson, C.A.Murillo and M.Bochmann, 6<sup>th</sup> Edition, Wiley Interscience, N.Y (1999).
6. Inorganic chemistry, J.E. Huheey, K.A.Keiter and R.L.Keiter 4<sup>th</sup> Edition Harper Cottens College Publications (1993).
7. The Chemistry of MetalCluster Complexes. D.F Shriver, H.D.Kaerz and R.D. Adams(Eds), VCH, NY (1990).
8. Inorganic chemistry, Keith F.Purcell and John C.Kotz, Holt-Saunders International Editions. London (1977).
9. Bioinorganic Chemistry, I.Bertini, S.J.Lippard and S.J.Valentine, Viva Low-Priced Student Edition, New Delhi (1998).
  - a. Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, W.Kain and B.Schwederski, John Wiley and Sons, NY (1999).
10. Bioorganic Chemistry – Dugas.
11. Analytical Chemistry-An Introduction, Skoog, West, Holler and Crouch. Saunders College Publishing.
12. Principles of Instrumental analysis, Skoog and Leary, Saunders College Publishing.
13. International series of Monographs, Vol.53: Photoelectron Spectroscopy, Edited by D.Betteridge 1972.
14. Structural methods in inorganic chemistry, E.A.V.Ebsworth.

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P. Jeeva

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15. Solid state and its applications by A.R. West.
16. New directions in solid state Chemistry. J. Gopalakrishnan and C. N. R. Rao.
17. Principles of the solid state by HV Keer.

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DEPARTMENT OF CHEMISTRY  
PALAMURU UNIVERSITY, MAHABUBNAGAR, TELANGANA

Ph.D. Course Work Syllabus

Paper-II: Organic Chemistry Specialisation

(Effective from Academic year)

(Approved in the PG Board of studies held on )

Marks:100

**UNIT-I: New Techniques and concepts in Organic Synthesis**

Ramachary -Reductive coupling, Ramachary-Bressy-wang cycloaddition, Click Chemistry, Passerini reaction, Ohira -Bestmann reaction, Baldwin rules, Thorpe-Ingold Effect, Organocatalysis - Proline (example-synthesis of Wieland-Miescher ketone and synthesis of chiral  $\beta$ -hydroxycarbonyl compounds), Mc Millans catalyst (Iminium ion mediated metal free asymmetric catalysis - Example Diels-Alder reaction), Organocatalytic epoxidation of cinnamaldehyde using diarylprolinol.

**UNIT-II: Asymmetric Synthesis: Introduction, Stereoselectivity**

**Asymmetric induction:** Oppolzer auxiliaries; Sharpless asymmetric aminohydroxylation, Shi epoxidation, Noyori's asymmetric hydrogenation, Mukaiyama aldol reaction, chiral pool strategy, synthesis of R and S-Sulcatol, methyl mycaminose from S-Lactic acid.

**Retrosynthesis:** Introduction,

**Selectivity:** Introduction, chemoselectivity- retrosynthesis of Lipstatin; regioselectivity-retrosynthesis of Gingerol; stereoselectivity- aldol reaction-anti and syn selective aldol reactions, retrosynthesis of Juvabione, Retrosynthesis of pancratistatin

**Aromatic compounds-ortho strategy:** Introduction, ortholithiation-anionic Fries rearrangement.

**One and two group C-C, C-X disconnections:** Introduction, retrosynthesis of Rogeltime, linalool and Doxipicmine.

**Reconnections:** Introduction, polarity reversal, synthesis of 1,2 and 1,4-dicarbonyl compounds.

**UNIT-III: Spectroscopic applications of Organic compounds.**

**Differentiation of possible isomers:** i)  $C_9H_{10}O_2$  - Number of possible isomers and their detection by  $^1H$ -NMR spectra. ii) Hydroxycinnamic acid-number of possible isomers and their detection.

**Differentiation of pair of isomers:** Differentiation of isomers using different spectra:

**IR spectra:** (i) 3-Phenylpropanaldehyde and Propiophenone (ii) 4-ethylaniline, 4-methyl-N-methylaniline and N, N-dimethylaniline.

**UV spectra:** (i) Propiophenone and phenylacetone (ii) levopimaric and abietic acid.

**$^1H$ -NMR Spectra:** (i) Vinyl acetate and Methyl acrylate (ii)  $\alpha$ - pinene and  $\beta$ -pinene.

**$^{13}C$ -NMR spectra:** (i) 1-pentene and 2-pentene (ii) vinyl acetate and methyl acrylate.

**Mass spectra:** (i) N, N- dimethylpropanamide and N-methylbutanamide (ii)  $\alpha$ -ionone and  $\beta$ -ionon (iii) Cyclohexylpropane and 1,2,4-trimethylcyclohexane (iv) Pyrazole and imidazole (v) Pyridazine, Pyrimidine and Pyrazine.

**All spectral data (IR, UV,  $^1H$ ,  $^{13}C$  and Mass spectra) of given examples:** paracetamol and p-methoxybenzamide.

**$^{13}C$ -NMR spectroscopy:** Sucrose (DEPT), Piperine and Morphine.

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**Quantitative estimation:** Quantitative estimation of APC tablets by  $^1\text{H-NMR}$  Spectroscopy.  
Determination of absolute configuration of enantiomers by Mosher's method.  
**2D- NMR spectroscopy:** principle – Homo-2D- J-resolved and hetero- 2D-J-resolved spectroscopy, Homo- COSY, TOCSY, Hetero-COSY, HMQC, HMBC, NOESY and 2D-Inadequate techniques by taking 1-iodobutane as an example. HOMO COSY of sucrose, Hetero-COSY, HMQC, HMBC, 2D-Inadequate of Ipsenol, TOCSY of methoxybutane, Homo-COSY and Hetero-COSY of Thymol.  
**Interpretation of the structure of natural products using spectral data (IR, UV, NMR & Mass):** Camphor,  $\beta$ -carotene, caffeine, penicillin-G, adenosine and cis-jasmone.

#### UNIT-IV: Green Chemistry and Biological Evaluation

**Green Chemistry:** Atom efficiency, E-factor calculation, Effective mass yield, Renewable feed stocks, Green solvents ( $\text{H}_2\text{O}$ , ionic liquids and supercritical  $\text{CO}_2$ ) and their applications in organic synthesis, biocatalysts in organic synthesis, Combinatorial green chemistry. Solvent free synthesis - preparation of  $\beta$ -lactams, pyrroles, quinolines. Biomimetic, multifunctional reagents, co crystal controlled solid state synthesis Green Synthesis of the following compounds: adipic acid, catechol, disodium imino-diacetate (alternative to Strecker synthesis)  
**Biological Evaluation:** *In-vivo* and *In-vitro* studies. Cell line assay, Enzyme inhibition, Toxicity testing, cell viability assay, High through put screening. Explanation for  $\text{IC}_{50}$ ,  $\text{EC}_{90}$ ,  $\text{LD}_{50}$ ,  $\text{ED}_{50}$ ,  $\text{Ki}$ ,  $\text{MIC}$ , Zone of inhibition studies. Ethical issues and regulatory affairs.

#### References:

1. Matlack, A.S. Introduction to Green Chemistry, Marcel Dekker (2001).
2. Cann, M.C. & Connely, M.E. Real-World cases in Green Chemistry, American Chemical Society, Washington (2000).
3. Ryan, M.A. & Tinnesand, M. Introduction to Green Chemistry, American Chemical Society, Washington (2002).
4. Lancaster, M. Green Chemistry: An Introductory Text RSC Publishing, 2nd Edition, 2010.
5. Organic Chemistry Jonathan Clayden, Nick Greeves and Stuart Warren
6. Organic Synthesis – The disconnection approach by S Warren
7. Organic Synthesis: Strategy and control by Paul Wyatt and Stuart Warren
8. Fundamentals of Asymmetric synthesis by G, L, David Krupadanam
9. Organic Synthesis by Michael B Smith
10. Principles of Medicinal Chemistry- Foye
11. An Introduction to Medicinal Chemistry Graham L Patric

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DEPARTMENT OF CHEMISTRY  
PALAMURU UNIVERSITY, MAHABUBNAGAR, TELANGANA

Syllabus for Ph. D. Course Work

Paper – II: Physical Chemistry Specialization.

(Effective from 202 - 202 Academic year)

(Approved in the P.G Board of Studies held on )

Marks:100

### UNIT-I: HETEROGENEOUS CATALYSIS

**Heterogeneous catalysis:** Broad categories of catalysis – metal, bimetal, semiconductors, insulators, zeolites, oxides and nano materials.

**Preparation of metal catalysts:** Supported metal catalysts and non-metallic catalysts.

**Characterization of catalysts:** Surface area by BET method. Determination of pore volume and pore size distribution by BJH method. Pore size and specificity of catalysts. Surface acidity of catalyst & determination of surface acidity by indicator method, IR spectroscopic method and TPD method.

**Steps in heterogeneous catalyzed reactions:** Catalytic activity – the determining factors. Structure sensitive and structure insensitive catalysts. Mechanism of surface – catalyzed reactions. The Langmuir – Hinshelwood and the Eley – Rideal mechanisms. Rate constants and activation energies of surface reactions.

**Introduction to Phase – transfer catalysts (PTC):** Principles of phase – transfer catalysts. PTC classification. Role of water in phase – transfer catalyzed reactions. Factors influencing the rate of PTC reactions. Inverse phase transfer catalysis.

### UNIT –II: FUNCTIONAL POLYMERS

Smart materials – uses of smart materials in sensing devices and communication networks.

**Conducting polymers:** Electrically conducting polymers and their uses (polyanilines, polypyrrole, polyacetylene and polythiophene). Photoconductive polymers. Liquid crystal polymers-smectic, nematic and cholesteric structures.

**Ionic exchange polymers:** Cationic and anionic exchange polymers and their uses. Eco-friendly polymers. Poly lactide from corn derived dextrose, PHB etc.

Membrane separation. Filtration - micro, ultra and nanofiltration. Separation of gases – permselectivity and gas permeability of representative polymers. Liquid separation – dialysis, electro osmosis and reverse osmosis. Fire retarding polymers, photonic polymers. Interpenetrating networks (IPN), polymers in photo lithography.

Polymers in biomedical applications – artificial organs and controlled drug delivery.

**Emerging polymers:** PTTC – (poly tri methylene tetra phthalate). Nylon 4,6 (Stanyl) – their structures, properties and uses.

### UNIT-III: ELECTRO CHEMISTRY

**Electrode- electrolyte interface:** The electrical double layer. The Helmholtz-Perrin parallel-plate model, the Gouy-Chapman diffuse-charge model and the stern model.

**Corrosion:** Electrochemical mechanism of corrosion. Types of corrosion, various methods of corrosion control.

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**D.C Polarography:** Dropping mercury electrode-polarography Instrumentation-Polarogram. Types of limiting Currents: Adsorption, Diffusion, Kinetic. Ilkovic equation and its consequences. Applications of polarography. Determination of stability constant of complex.

**Cyclic voltammetry:** Principle, instrumentation. reversible and irreversible cyclic voltammograms. Applications. Cyclic voltammetric study of insecticide parathion.

**Electro-Organic synthesis:** Electro chemical reduction of carboxylic acids, Electrochemical reduction of nitro compounds.

**Anodic oxidation of metals:** Characteristics of anodic oxide films. Instrumentation – break down voltage. Industrial applications of anodic oxide films.

#### UNIT IV: MATERIALS SCIENCE AND MOLECULAR MODELING

Preparative methods of inorganic solids: Ceramic, Co-precipitation, sol-gel, chemical vapor transport.

**Characterization techniques of inorganic solids:** X-ray powder diffraction (XRD), transmission electron microscopy (TEM) and X-ray photoelectron spectroscopy (XPES).

**Composites:** Classification, fiber reinforced composites-influence of fiber length.

**Nanomaterials:** Preparation by sol-gel and hydrothermal methods. Characterization by powder XRD-Scherer's equation and general application.

**Molecular modeling:** QSAR parameters – Physiochemical parameters - Lipophilicity – Electronic parameters. Steric parameters, effect of electronic and steric parameters on lipophilicity. Hansch analysis, significance of slopes and intercepts in Hansch analysis. QSAR- 2D, 3D.

Case study - on Pyranenamine. Achievements of QSAR - Forecasting biological activity, Selection of proper substituents, bioisosterism, drug receptor interactions and pharmacokinetic Information - Introduction to database similarity Search – Alignment; Alignment methods- Pair-wise alignment: Multiple Sequence Alignment – Homology Modeling – Energy minimization methods –Active site Identification –Virtual Screening–Small molecule Building -Docking Algorithms – Docking Analysis

#### References:

##### Catalysis:

1. Principles of Heterogeneous Catalysis in practice, G.C.C Bond, Oxford Publishing
2. Heterogeneous Catalysis, C. Satterfield, McGraw Hill
3. Catalysis. Principles and applications, edited by B. Vishwanathan, S. Sivasanker & A. V. Rama Swamy, Narosa Publishing House
4. Catalysis J.C. Kuriacose, Macmillan
5. Phase Transfer Catalysis, Fundamentals, Applications and Industrial perspective. C. M. Stark, C. Liotta & M. Halpern, Academic Press
6. Phase Transfer Catalysis, E. V. Dehmlow & S.S. Dehmlow, Verlag chemie. Weinheim
7. Phase Transfer Catalysis in Organic synthesis, W. P. Weber & G.W. Gokel. Springer

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*A. Radwan*  
*Burhan*

*Erasmus*



### Functional Polymers:

8. Textbook of Polymer Science, F.W. Billmeyer Jr. John Wiley & sons
9. Polymer Science, V.R. Gowarikar, N.V. Viswanathan & J. Sreedhar, Wiley Eastern
10. Contemporary Polymer Chemistry, H.R. Alcock & F.W. Lambe, Prentice Hall
11. Physics and Chemistry of Polymers, J.M.G. Cowie Blackie Academic and professional
12. Polymer Chemistry, B. Vollmert
13. Physical Chemistry of Polymers, A. Tagers, Mir Publishers
14. Introduction to Polymer Chemistry, By Charles E Carraher Jr (Taylor- Francis)

### Electro Chemistry:

15. Modern ElectroChemistry 2A & 2B, J.O.M. Bockris & A.K. N. Reddy, Plenum publishers
16. Introduction to ElectroChemistry, S. Glasstone
17. Industrial ElectroChemistry, D. Pletcher, Chapman & Hall
18. Fundamental principles of Modern Electroplating, Lowenheim, John Willey
19. Principles of Polarography, Heyrovsky.
20. Principles of Polarography, Kapoor.
21. Modern Electroanalysis methods, edited by C. Charlot, Elsevier Company.
22. Principles of Instrumental analysis, Skoog, Holler and Nieman, Harcourt Asia PET Ltd.
23. Analytical Chemistry- An Introduction, Skoog, West, Holler and Crouch. Saunders College Publishing.
24. Principles of Instrumental analysis, Skoog and Leary, Saunders College Publishing.

### Material Science:

25. Solid state and its applications by A.R. West.
26. New directions in solid state Chemistry. J. Gopalakrishnan and C. N. R. Rao.
27. Principles of the solid state by HV Keer.

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MODEL PAPER  
FACULTY OF SCIENCE  
Ph.D. Course Work Examination  
Subject: CHEMISTRY  
Paper- I: Research Methodology  
(Common to all Specializations)

Code No:

Time: 3 Hours

Max. Marks: 100

Note: Answer all questions from Section- A and Section- B. Each question carries 10 marks in Section- A and 15 marks in Section- B.

Section-A ( $4 \times 10 = 40$  Marks)  
(Short Answer Type)

1. a)  
b)
2. a)  
b)
3. a)  
b)
4. a)  
b)

Section-B ( $4 \times 15 = 60$  Marks)  
(Essay Answer Type)

5. a)  
b)

OR

- c)  
d)
6. a)  
b)

OR

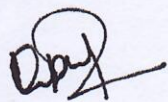
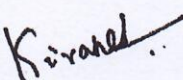
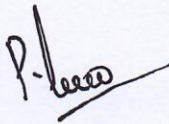
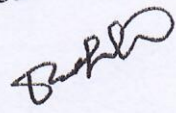
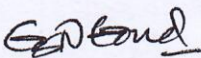
- c)  
d)
7. a)  
b)

OR

- c)  
d)
8. a)  
b)

OR

- c)  
d)

Margal  Kiran  P.  A. Padmal   
S. 



MODEL PAPER  
FACULTY OF SCIENCE  
Ph.D. Course work Examination  
Subject: CHEMISTRY  
Paper- II  
(Title of Research Specialization)

Code No:

Time: 3 Hours

Max. Marks: 100

Note: Answer all questions from Section - A and Section - B. Each question carries 10 marks in Section - A and 15 marks in Section - B.

Section-A ( $4 \times 10 = 40$  Marks)  
(Short Answer Type)

1. a)  
b)
2. a)  
b)
3. a)  
b)
4. a)  
b)

Section-B ( $4 \times 15 = 60$  Marks)  
(Essay Answer Type)

5. a)  
b)

OR

- c)  
d)
6. a)  
b)

OR

- c)  
d)
7. a)  
b)

OR

- c)  
d)
8. a)  
b)

OR

- c)  
d)

K. Gijit

Apur

Kiransh

Kloozah  
G. S. S. S.

P. S. S.

A. Padmavati  
B. S. S.