MAHATMA GANDHI UNIVERSITY
NALGONDA – 508 254

DEPARTMENT OF CHEMISTRY

Syllabus for Ph.D. Course Work

Paper- I : (COMMON TO ALL BRANCHES)

Unit-I: SYMMETRY OF MOLECULES & REACTION MECHANISMS OF TRANSITION METAL COMPLEXES

15 hrs

i) Symmetry of Molecules: Concept of Symmetry in Molecules – Symmetry Operations & Symmetry,Elements: Rotational Axis of Symmetry and Types of Rotational Axes, Plane of Symmetry and types of Planes, Improper Rotational Axis of Symmetry, Inversion Center and Identity Element – More about Symmetry Elements – Molecular Point Groups: Definition and Notation of Point Groups, Classification of Molecules in to C1, Cs , Ci, Cn, Cnv, Cnh, Cv, Dn, Dnh, Dnd, Sn (n = even), , Td, , Oh and Ih Groups. Properties of a group-sub group.

ii) Reaction mechanisms of transition metal complexes:
Ligand substitution reactions: Energy profile of a reaction- Transition state of Activated complex. Types of substitution reactions (SE,SN, SN1, SN2).

Ligand substitution reactions in octahedral complexes*:* Acid hydrolysis reactions, Factors effecting Acid Hydrolysis, Base Hydrolysis, Conjugate Base Mechanism, Evidences in favour of SN1CB Mechanism. Substitution reactions without Breaking Metal-Ligand bond.

Ligand Substitution reactions in Square-Planar complexes: Mechanism of Substitution in Square-Planar complexes- Trans-effect, Grienberg's Polarization theory and π - bonding theory – Applications of Trans-effect in synthesis of Pt (II) complexes.

Electron Transfer Reactions (or Oxidation-Reduction Reactions) in Coordination compounds: Mechanism of One-electron Transfer Reactions: Atom (or group) Transfer or Inner Sphere Mechanism, Direct electron Transfer or Outer Sphere Mechanism.

UNIT- II: STRATEGIES IN ORGANIC SYNTHESIS **15 hrs**

i) Oxidations: Swern, Prevost and Woodward oxidations.
ii) Reductions: Birch reduction, Reduction with LiAlH4 , NaBH4 , BH3, AlH3, and tri-n-butyl tin hydride.

iii) Organo- metallic reagents: Use of Organo lithium, Silicon and boron reagents in Organic synthesis.
iv) Modern Organic Synthetic Reactions: Aza-Cope and Aza-Wittig reactions, Baylis-Hillman reaction, BINAL and BINAP assisted reactions, Buchwald-Hartwig coupling, Click reaction, Grubb's catalyst and RCM olefin metathesis, Heck reaction, Julia- Lythgoe olefination, Mukayama aldol reaction, Mitsunobu reaction, McMurray reaction, Peterson's stereoselective olefination, Suziki coupling.

UNIT - III: CHEMICAL KINETICS & PHOTO CHEMISTRY **15 hrs**

Chemical Kinetics: Structure-Reactivity relationships- Linear free energy relationships. Hammett equation – The substituent constant(σ) and exalted sigma values. The Reaction constant (ρ) and the importance of rho value in arriving at the mechanism of reactions. Deviations from Hammett correlations. Taft equation and Taft four parameter equation. The Swain – Scott equation- Correlations for nucleophillic reactions. The Edward equation. The reactivity-selectivity principle and the isoselectivty rule. The intrinsic barrier and Hammond's postulate.

Photo Chemistry: Formation of excimers and exciplexes –Quantum yields. Electronically excited states- singlet and triplet states. Uni molecular decay of the excited state- internal conversion, inter system crossing, fluorescence and phosphorescence. Principles of energy transfer- photosensitization. Flash photolysis and it's applications . Organic photochemistry. Properties of (n, ||*) and (||, ||*) states. Photochemistry of alkenes: Cis-trans isomerisation, di-||- methane rearrangement. Photochemistry of carbonyl compounds: i) Norrish type-I reactions. Photoreduction and photooxidation.ii) Norrish type-II reactions. Addition of carbonyl to carbon-carbon multiple bonds (Paterno-Buchi) reaction. Barton reaction. Singlet oxygen – photo oxidation and reactions with C=C compounds. $Ru(bpy)_3^{+2}$ as sensitizer for photo redox reactions. Photochemical cleavage of water.

UNIT-IV: PRINCIPLES OF SPETROSCOPY **15 hrs**

i) IR Spectroscopy: Introduction, Principles, Characteristic vibrational frequencencies of functional groups, Fermi resonance, Effect of hydrogen bonding on vibrational frequencies.
ii) Electronic spectroscopy: Introduction, Principles and Wood -Ward Fisher rules.
iii) NMR Spectroscopy (1H NMR): Introduction, Principles, factors effecting the chemical shifts, spinspin coupling, first order spectra.
iv) Mass Spectrometry: Introduction, Principles, use of isotopic peaks, salient feature of fragmentation of organic compounds, McLafferty rearrangements, retro Diels-Alder fragmentation and ortho effects. Simple problems on structure determination based on the above spectral methods.
Atomic Absorption Spectroscopy (AAS): Principles of AAS– flame AAS and furnace AAS, sensitivity and detection limits in AAS, interferences – chemical and spectral, evaluation methods in AAS and applications in qualitative and quantitative analysis.
Atomic Emission Spectroscopy (AES): Principles of AES, Instrumentation, evaluation methods and application in quantitative analysis.

REFERENCE BOOKS:

Unit- I: Symmetry of molecules & Reaction mechanisms of transition metal complexes

1. Symmetry and Spectroscopy of Molecules, K. Veera Reddy, Second Edition, New Age International (P) Limited Publishers (2009)
2. Chemical Applications of Group Theory, F. A. Cotton, 3rd edition, Wiley NY (1990)
3. Symmetry and Group Theory In Chemistry, Mark Ladd, Harwood Publishers, London (2000)
4. Symmetry Through the Eyes of a Chemist, I. Hargittai and M. Hargittai, 2nd Edition, Plenum Press, NY (1995)
5. Reaction mechanism in transition metal complexes .K.Veera Reddy New Age International (P) Limited Publishers.

UNIT- II: Strategies in Organic Synthesis

1. Some modern methods of organic synthesis by W Carruthers
2. Guidebook to organic synthesis, by R K Meckie, D M Smith & R A Atken
3. Organic synthesis by O House
4. Organic synthesis by Michael B Smith
5. Reagents for organic synthesis, by Fieser & Fieser, Vol 1-11(1984)
6. Organic synthesis by Robert E Ireland
7. Organic Synthesis - The disconnection approach by S Warren
8. Organic Synthesis by C Willis and M Willis
9. Handbook of reagents for organic synthesis by Reich and Rigby, Vo I, IV
10. Problems on organic synthesis by Stuart Warren
11. Total synthesis of natural products: the Chiron approach by S.Hanessian
12. Organic chemistry Claydon and others 2005
13. Name Reactions by Jie Jack Li
14. Reagents in Organic synthesis by B.P.Mundy and others.
15. Tandem Organic Reactions by Tse-Lok Ho.

UNIT - III: Chemical Kinetics & Photo Chemistry

1. Chemical Kinetics, K. J. Laidler, McGraw Hill
2. Kinetics and Mechanism, A. A. Frost & R. G. Pearson, John Wiley & sons
3. Kinetics and Mechanism of Chemical Transformations, J. Rajaraman & J. Kuriacose, McMillan
4. Chemical Kinetics and Reaction Mechanisms, J. H. Espenson, McGraw Hill
5. Physical Organic Chemistry, N. S. Isaacs, ELBS
6. The Physical basis of Organic Chemistry, Howard Maskill, Oxford University Press
7. Molecular Photochemistry, N. J. Turro, W. A. Benzamin
8. Fundamentals of Photochemistry, Rohatgi-Mukherjee, Wiley Eastern
9. Essentials of Molecular Photochemistry, A. Gilbert & J. Baggott, Blackwell Science
10. Introduction to Molecular Photochemistry, C. H. J. Wells, Chapman and Hall

11. Molecular Reactions and Photo chemistry by Depuy and Chapman

UNIT-IV: Principles of Spectroscopy

1. Fundamentals of Molecular Spectroscopy, Banwell and McCash.
2. Introduction to Molecular Spectroscopy, G.M. Barrow
3. Absorption Spectroscopy of Organic Compounds, J.R. Dyer
4. Biochemistry: Hames and Hooper.
5. Spectroscopic identification of organic compounds by R.M.Silverstein. G.C.Bassler and T.E.Morrill
6. NMR-A multinuclear introduction by William Kemp
7. Organic Spectroscopy by William Kemp
8. Spectroscopic methods in Organic chemistry by DH Williams and I Fleming
9 . Modern NMR techniques for chemistry research by Andrew B Derome
10. NMR in chemistry - A multinuclear introduction by William Kemp
11. Spectroscopic identification of organic compounds by P S Kalsi
12. Introduction to organic spectroscopy by Pavia
13. Carbon-13 NMR for organic chemists by GC Levy and O L Nelson
14. Principles of Instrumental Analysis, Skoog, Holler and Nieman.
15. Instrumental Techniques for Analytical Chemistry, Frank Settle.
16. Principles of Analytical Chemistry, M. Valcarcel

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Syllabus for Ph.D. Course work

Paper- II: Organic Chemistry Specialization

UNIT-I : NMR Spectroscopy: 15 hrs

a) ^{13}C NMR (CMR) Spectroscopy: Principles involved and different types of CMR spectra, Chemical shifts and coupling in CMR. Applications of CMR spectroscopy to structure determination, stereochemistry, reaction mechanisms and dynamic processes in organic molecules. 13C NMR spectral editing techniques. Principles and applications of APT, INEPT and DEPT techniques.

b) 2D- NMR Spectroscopy: Principles and applications of the following 2D- NMR experiments.
i) HOMO and Heteronuclear J resolved spectroscopy ii) HOMO COSY and TOCSY
iii) HETERO COSY , HMQC and HMBC iv) NOESY v) INADEQUATE

UNIT-II: Natural Product Chemistry: 15 hrs

a) IR, UV, 1H, 13C , 2D- NMR and mass spectral studies of the following classes of Natural Products:
i) Coumarins ii) Flavones iii) Isoflavones iv) Flavanones v) monoterpenes vi) Quinoline and isoquinoline alkaloids (cusparine and papaverine)
b) Structure elucidation, synthesis and stereochemistry of the following.
i) Taxol ii) Vincaleucoblastine iii) Reserpine iv) Rotenone.

Unit -III : Modern Concepts of Organic Chemistry and Green Chemistry: 15 hrs

a) New Techniques and concepts in organic synthesis. i) Combinatorial synthesis ii) Phase transfer catalysis iii) Tandem synthesis iv) Mosher's method for configuration determination v) Baldwin rules vi)Kahne's glycosidation vii) Methods of oligonucleotide synthesis.

b) Green Chemistry: Introduction, principles of green chemistry, Different approaches to green synthesis: Microwave and Ultrasound assisted organic synthesis, Solid phase and aqueous phase organic synthesis.

UNIT-IV: Synthetic strategies and Asymmetric synthesis. 15 hrs

a) Design of Organic synthesis: Terminology, Retrosynthesis, FGI, disconnection, synthon synthetic equivalent, protecting groups, chemoselectivity, regioselectivity and stereoselectivity. Linear and convergent strategies, Use of disconnection approach in the synthesis of multistriatin, Warfarin and α-bisabolene.

b) Asymmetric Synthesis: Terminology, concepts of prochirality, enantioselectivity and diastereo selectivity. Methods for determination of enantiomer purity: Polarimeter, 1H-NMR and HPLC methods.
i) Asymmetric hydrogenation using chiral Wilkinson biphosphine and Noyori catalysts; approaches to L- DOPA and L-α- amino acids.
ii) Asymmetric aldol reaction and asymmetric Diels-Alder reaction.
iii) Chiron approach to stereoselective synthesis of (-) PGE2 and (-) shikimic acid.

REFERENCES:

NMR Spectroscopy:

1. Spectroscopic identification of organic compounds by RM Silverstein, G C Bassler andT B Morrill
2. Organic Spectroscopy by William Kemp
3. Spectroscopic methods in Organic chemistry by DH Williams and I Fleming
4. Modern NMR techniques for chemistry research by Andrew B Derome
5. NMR in chemistry - A multinuclear introduction by William Kemp
6. Spectroscopic identification of organic compounds by P S Kalsi
7. Introduction to organic spectroscopy by Pavia
8. Carbon-13 NMR for organic chemists by GC Levy and O L Nelson

Natural Product Chemistry:

1. Textbook of organic chemistry, Vol II by I L Finar
2. Chemistry of natural products, Vol 12, by Atta-Ur-Rahman
3. An introduction to the chemistry of terpenoids and steroids by William templeton
4. Systematic identification of flavonoid compounds by Mabry & Markham
5. Steroids by Fieser and Fieser
6. Alkaloids by Manske
7. Alkaloids by Bentley
8. The chemistry of terpenes by A Pinder
9. The terpenes by Simenson
10. Terpenoids by Mayo
11. Alkaloids by Pelletier
12. Total synthesis of Natural Products by Apsimon Vol 1-5
13. Biosynthesis by Geismann
14. Principles of organic synthesis 3rd Ed.R O C Norman and J M Coxen
15. One and two dimensional nmr spectroscopy by Atta Ur Rahman
16. Classics in total synthesis K C Nicolaou and E J Sorenson

Modern Concepts of Organic Chemistry and Green Chemistry:

1. Some modern methods of organic synthesis by W Carruthers
2. Guidebook to organic synthesis, by R K Meckie, D M Smith & R A Atken

3. Organic synthesis by O House
4. Organic synthesis by Michael B Smith
5. Reagents for organic synthesis, by Fieser & Fieser, Vol 1-11(1984)
6. Organic synthesis by Robert E Ireland
7. Organic Synthesis - The disconnection approach by S Warren
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11. Total synthesis of natural products: the Chiron approach by S.Hanessian
12. Organic chemistry by Claydon and others 2005
13. Name Reactions by Jie Jack Li
14. Reagents in Organic synthesis by B.P.Mundy and others.
15. Tandem Organic Reactions by Tse-Lok Ho
16. Organic synthesis in water. By Paul A. Grieco Blackie.
17. Green chemistry, Theory and Practical, Paul T.Anastas and John C.Warner.
18. New trends in green chemistry By V.K.Ahulwalia and M.Kidwai.
19. Organic Synthesis: Special techniques. V.K.Ahulwalia and Renu Aggarwal

Synthetic strategies and Asymmetric synthesis.

1. Stereochemistry: Conformation & Mechanism by P S Kalsi
2. Stereochemistry of Carbon compounds by Ernest L Eliel
3 . Stereoselectivity in organic synthesis by R S Ward.
4. Asymmetric synthesis by Nogradi
5. Asymmetric organic reactions by it) Morrison and HS Moscher
6. Stereo differentiating reactions by Izumi
7. Some modern methods of organic synthesis by W Carruthers
8. Guidebook to organic synthesis, by R K Meckie, D M Smith & R A Atken
9. Organic synthesis by Michael B Smith
10. Organic Synthesis by C. Willis & M. Willis
11. Total Synthesis of natural products: the Chiron approach by S. Hanessian
12. Organic Synthesis- The disconnection approach by S. Warren
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14. Organic Chemistry by Claydon and others.

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Syllabus for Ph.D. Course Work

Paper- II : Inorganic Chemistry Specialization

Bonding in metal complexes, Spectroscopic Applications, Supramolecular, Organometallic and Bio-inorganic Chemistry

Unit-I: Bonding in metal complexes, Electron absorption Spectroscopy (15 hrs)

Molecular Orbital Theory of Metal Complexes: Symmetry Classification of Metal and Ligand 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 for Octahedral, Tetrahedral and Square Planar Metal Complexes with Sigma (σ) and Pi (π) Bonding Contribution from the Ligands.

Electron absorption spectroscopy: Effect of weak cubic crystal fields on S,P,D and F terms- Orgel Diagrams. **S**election 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 3dn Metal ions – Calculation of 10Dq Values, Racah Parameter.

Unit-II: IR, Raman, NMR and ESR (15 hrs)

IR and Raman: Symmetry Based Selection Rules of Infrared 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.

Multinuclear NMR: Characteristic Nuclear Properties of 1H, 13C, 19F, 31P and 15N – Reference standards- Ranges of Chemical Shifts –Use of Chemical Shifts and Coupling Constants for the structure determination of simple inorganic and Coordination Compounds containing one or more of 1H, 13C, 19F, 31P and 15N nuclei.Examples; (1)1H-NMR: Pt HCl(PEt3)2 , Pt (NH3)3(CH3)3, BH_4^- , [h7C7H7Mo(CO)3]+ , B2H6; (2) 19F- NMR: PF5, BF_4^-, SF4; (3) 31P-NMR: H3PO2, H3PO3, H3PO4, [Rh (PPh3)3 Cl3], [Mo(CO)3(PPh3)3], [Rh (PPh3)3 Cl] , ATP. (4) 13C-NMR: [h4 C8H8 Ru(CO)3], Fe(CO)5, Fe2(CO)9, Fe3(CO)12, [13C 15N Co(DH)2Pyridine].

ESR of Metal Complexes: Principle- Selection Rules –. g value and its significance, Interpretation of g in cubic , axial and rhombohedral geometries. Factors affecting g values. Calculation of g values with simple examples. Intensities of '$g_{\parallel}$ and $g_{\perp}$ peaks . Evidence for Metal-Ligand Bond Covalency-Cu(II)- Bis –Salicylaldimine. Co3(CO)9Se, [(NH3)5CoO2 Co

(NH3)5]5+, Cu(II)- diethyldithio phosphinate, Vanadyl dithio phsphinate, Copper(II) tetraphenyl porphyrin, Co(II)- phthalocyanine, K2[IrCl6].

Unit-III: Supramolecules and Organo metallic Catalysis (15 hrs)

Supramolecular chemistryHost – Guest chemistry : Definition and different types of host and guests with examples – types of non covalent interactions – binding constants of host guest complex and thermo dynamics involved in it – designing principles of host. **Cation guest binding** – binding between metal cations and macro cycles – chelate and cryptate effects – relationship between cavity size of host and cation radius and stability of resultant complexes – binding of macro cycles having secondary binding sites – **Anion guest binding** – different hosts for anionic guests capable of binding through electro static interactions, hydrogen bonds, lewis acidic hosts – enhancement of binding strength using more than non covalent interactions – **Neutral guest binding –** binding of neutral guest using hydrogen bonding, π - π stacking, hydrophobic effect and charge transfer interactions – simultaneous binding of cation and anion guests – cascade approach, individual binding sites and zwitter ions approach –present and future applications – phase transfer agents – separation of mixtures – molecular sensors – switches and molecular machinery.

Catalytic role of Organometallic Compounds: Oxidative addition and Reductive Elimination : Stereochemistry and Mechanism of Oxidative Addition – Insertion Reactions – Hydrogenation of Olefins –Transfer Hydrogenation – Hydrosilation of Olefins – Isomerisation of Olefins – Ziegler – Natta Polymerization of Olefins – Oligomerization of Butadiene . Alkene Metathesis. Oxidation of Olefins to Carbonyl Compounds – Oxidation of Hydrocarbons to Alcohols and Acids – Oxidation of Aldehydes. Reactions of Carbon monoxide and Hydrogen : Hydroformylation – Carbonylation –Syngas-Water gas shift Reaction (WGS) – Reactions of Syngas. Applications of Metal Clusters in Catalysis : Hydroformylation of Ethylene using [HRu3(CO)11]– , Hydrogenation of Olefins. Use of [Fe6C(CO)16] as a model for Fischer – Tropsch process.

Unit-IV: Bio inorganic Chemistry (15 hrs)

Role of metal ions in biology – four basic principles in the biological selection of elements – brief survey of metal ions in biological system – effect of metal ion concentration and physiological effect.

Cobalt enzymes : chemistry, biochemistry and medicinal aspects of vit B12 – structure of vit B12 –various forms – Base 'On' and Base 'Off' and His 'On' or His 'Off' forms – complete and incomplete corrinoids – comparison of two biologically active forms of vit B12 – catalyzed reactions of vit B12 using coenzyme B and methyl cobalamin – biomethylation, methyl transfer to mercury and arsenic – vit B12 as drug transport vehicle – bio chemistry – functions of vit B12, symptoms and causes of vit B 12 deficiency, absorption and storage of vit B12 – historical events in the discovery of vit B 12.

Nickel enzymes : Urease – active site – mechanism of degradation of urea to carbon dioxide and ammonia.**Copper enzymes :** Substrate specific antioxidants – Cu, Zn superoxide dismutase – structure and catalytic mechanism. **Zinc enzymes :** Role of zinc in catalytic activities of carbonic

hydrase, carboxy peptidase and alkaline phosphate. **Vit B6 :** Various forms – mechanism of catalysed reactions – Dunothan hypothesis – role of metal ions in B6 catalytic activity.

Platinum complexes in cancer therapy: Discovery, applications and structure effect Relationships. Cis platin(cis Pt(NH3)2Cl2) mode of action. Drug resistance and DNA repair mechanism.

Physical effects of metal complex: DNA binding, unwinding, shortening and bending of the double helix. Biological consequences of platinum –DNA binding. Transition metal complexes as donor acceptor pairs. Non classical platinum antitumor+ agents.

REFERENCES & SUGGESTED BOOKS:

1. Symmetry and Spectroscopy of Molecules, K. Veera Reddy, Second Edition, New Age International (P) Limited Publishers (2009)
2. Chemical Applications of Group Theory, F. A. Cotton, 3rd edition, Wiley NY (1990)
3. Symmetry and Group Theory In Chemistry, Mark Ladd, Harwood Publishers, London (2000)
4. Symmetry Through the Eyes of a Chemist, I. Hargittai and M. Hargittai, 2nd Edition, Plenum Press, NY (1995)
5. Molecular Symmetry and Group Theory, Robert L. Carter, John Wiley & Sons (1998)
6. Group Theory for Chemists, G. Davidson, Macmillan Physical Science Series (1991)
7. Molecular Symmetry, Schoenland
8. Electronic Spectroscopy, A. B. P. Lever
9. Introduction to Ligand fields, B. N. Figgis Infrared and Raman Spectroscopy of Inorganic and Coordination Compounds, K. Nakamoto
10. Infrared spectroscopy of Inorganic Compound, Bellamy
11. Physical Methods in Chemistry, R. S. Drago, W.B. Saunders Co., 1977.
12. Chemical Structure and Bonding, R.L. Decock and H.B. Gray.
13. Physical Methods for Chemists, Russell S. Drago Second edition, Saunders ,College Publishing, 1992.
14. Comprehensive Coordination Chemistry, Vol 6.
15. Modern Coordination Chemistry, Lewis and Wilkins.
16. Organometallics-A Concise Introduction, Ch.Eischeinbroich and Salzer-VCH
17. Organotransition Metal Chemistry Fundamental Concepts and Applications, John Akio Yamamato, Wiley & Sons.
18. Homogeneous Catalysis by Metal Complexes, M M Taqui Khan and A E Martel
19. Applied Homogenous Catalysis with Organo Metallic Compounds Vol I & II, Boy Cornills and W A Herrmann – VCH
20. Homogenous catalysis, G W Parshall, John Wiley & Sons, New York
21. Inorganic elements in the Chemistry of life, Wolfgang Kaim & Brigette Schwederdki.
22. Bio inorganic Chemistry, Bertini, Lippard and Valentine, University Science Books, California USA, 1994
23. Principles Bioinorganic Chemistry., S J Lippard and Berg University Science Books, California USA, 1994
24. Biological Chemistry of Elements, J. J.R. Franstodasilva and R.J.P. Williams, aoxford University Press 1991
25. Metal ions in Biological Systems (series) Ed.H. Sigel Marcel Dekkar, New York
26. Inorganic Biochemistry, J.A. Cowan, VCH publishers 1993

27. Advances in Inorganic Biochemistry, edited by by G.L. Eichorn & Marzilli
28. Bioinorganic Chemistry, Vol-I edited by G. L. Eichorn

DEPARTMENT OF CHEMISTRY, MAHATMA GANDHI UNIVERSITY

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Paper- II: Physical Chemistry Specialization

UNIT-I : HETEROGENEOUS CATALYSIS (15 hrs)

Heterogeneous catalysis: Broad categories of catalysts – metals, bimetals, 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 catalysis (PTC*):* Principles of phase-transfer catalysis. 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: (15hrs)
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 – permeselectivity and gas permeability of representative polymers. Liquid separation – dialysis, electro osmosis and reverse osmosis. Fire retarding polymers, photonic polymers. Inter penetrating 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 : (15hrs)
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.

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 (15 hrs)

Preparative methods of inorganic solids: Ceramic, coprecipitation, 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 XRDScherer's equation and general applications.

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. 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

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. Ploymer Chemistry, B. Vollmert
13. Physical Chemistry of Polymers, A. Tagers, Mir Publishers
14. Introduction to polymer Chemistry, By Charles E Carraher Jr (Taylor- Frncis)

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 Wiley
19. Principles of Polarography, Heyrovsky.
20. Principles of Polarography, Kapoor.
21. Modern Electroanalytical methods, edited by C.Charlot, Elsevier Company.
22. Principles of Instyrumental analysis, Skoog, Holler and Nieman, Harcourt Asia PTE Ltd.
23. Analytical Chemistry-An Introduction, Skoog, West, Holler and Crouch, Saunders College Publishing.
24. Prinicples 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.
28. Materials science and engineering an introduction by W.D. Callister, Jr.

Molecular modeling:

29.Burger's medicinal chemistry and drug discovery. By Manfred E. Wolf.
30. Introduction to Medicinal chemistry. By Patrick.
31. Introduction to drug design. By Silverman
32. Comprehensive medicinal chemistry. Vol 1-5 By Hanzsch.
33. Principles of medicinal chemistry. By William Foye
34. Biochemical approach to medicinal chemistry. By Thomas Nogrady.
35. Pharmaceutical Chemistry and Drug synthesis By Roth and Kleeman
36. Drug design By E.J. Arienes
37. Jenkin's quantitative pharmaceutical chemistry By Knevel and Dryden
38. Recent advances in Bioinformatics By I. A. Khan and A Khanum
39. Computational chemistry By GH. Grant and WG. Richards
40. Molecular modelling By Hans Dieter Holtje and Gerd Folkers

41. Computational Chemistry by Jenson
42. Bio Informatics by Rastogi
43. The Science and practice of Pharmacy – Vol I and Vol II by Remington

MODEL PAPER

FACULTY OF SCIENCE

Code No:

Pre. Ph.D. Examination

Subject: **CHEMISTRY**

Paper- I

(Common to all branches)

Time: 3 Hours **Max. Marks : 100**

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

PART-A (4 × 10= 40 Marks)

(Short Answer Type)

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

PART-B (4 × 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)

MODEL PAPER

FACULTY OF SCIENCE

Code No:

Pre. Ph.D. Examination

Subject: **CHEMISTRY**

Paper- II

(Specialization)

Time: 3 Hours **Max. Marks : 100**

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

PART-A (4 × 10= 40 Marks)

(Short Answer Type)

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

PART-B (4 × 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)