ANNAMALAI UNIVERSITY

DEPARTMENT OF CHEMISTRY

Ph.D CHEMISTRY

SYLLABUS

ANNAMALAI UNIVERSITY
DEPARTMENT OF CHEMISTRY
Ph. D CHEMISTRY
PAPER I – RESEARCH METHODOLOGY

UNIT I: Introduction to Research Methodology

Objectives of research – Types of research – Significance of research. Research methods versus methodology – Research and scientific method – Criteria of good research – Problems encountered by researchers in India.
Problem selection – project proposal – funding agencies.

UNIT II: Literature Survey

Primary sources of journals and patents – Secondary sources – Listing of titles – Abstracts – Beilstein - Compendia and tables of information – Reviews – General treatises – Monographs and treatises on specific areas - Literature search – Information about a specific compound – Science citation index – Box to locate journals.

UNIT III: Thesis and Paper writing:

Conventions in writing – General format – Page and chapter format – Use of quotations and footnotes – Preparations of tables and figures – References – Appendices – Revising, editing and evaluating the final material – Proof reading – meanings and example of commonly used abbreviation.

UNIT IV: Data Analysis:

Precision and accuracy – Reliability – Determinate and random errors – Distribution of random errors – Normal distribution curve – Statistical treatment of finite samples – t test and F test - criteria for rejection of an observation – The Q test – Significant figures and computation rules – Data plotting – Least square analysis – Multiple linear regression - Significance of correlation coefficient.

UNIT V: Laboratory Safety:

General guidelines. Hygiene – Eye, foot, skin and hand protection – Safety rules - Equipment protection – Respiratory protective equipment – safety equipment – Leaking compressed gas cylinders – electrical safety. Fire – fire extinguishers. Laboratory injuries and treatment. Chemical spills – Mercury and Biohazardous – clean up procedure - Accident management - Disposal of chemicals and glass wares.

References:

1. C. R. Kothari, Research Methodology, New Age International Publishers. New Delhi, 2004.
2. R.A Day and A.L. Underwood, Quantitative analysis, Prentice Hall, 1999.
3. D.G Peters, J.M. Hayes and G.M. Hefige, A brief introduction to Modern chemical analysis, Saunders, 1976.

4. R. Gopalan, Thesis writing, Vijay Nicole Imprints Private Ltd., 2005.
5. R. Gopalan, P. S. Subramanian and K. Rengarajan, Elements of Analytical Chemistry, Sultan Chand and Sons, New Delhi, 2005.

PAPER II – SYNTHESIS AND CHARACTERIZATION OF ADVANCED MATERIALS

UNIT I: Surface characterization of Solids:

Study of surface electron spectroscopy, XPS, Auger electron spectroscopy, Scanning electron microscopy, Scanning tunneling microscopy, Atomic force microscopy, X-ray fluorescence, EDX.

UNIT II: Lasers

General principles of laser action – nature of stimulated emission – Resonators and pumping processes – population inversion – cavity mode characteristics – Q-switching mode locking – properties of laser light – beam width, intensity, coherence, monochromaticity – Gas lasers – CO_2, N_2, He-Ne lasers – liquid dye lasers – solid state lasers – nontunable and tunable – Ruby, Titanium sapphire, Nd:YAG – SHG - NLO phenomena – Excimer lasers – Intrinsic semiconductors – doped semiconductor – n-p junction – extrinsic semiconductors – Diode lasers – Difference between the LED and diode laser – Applications of laser in chemistry.

UNIT III: Synthesis of Nanomaterials

Common preparative methods; CVD, Sol-Gel, Attrition procedures – Carbon based nanomaterials : Synthesis of nanocarbon tubes – purification – mechanism of growth – Electronic structure – Transport properties – Mechanical properties – Nanotubes of other materials.

UNIT IV: Applications of Nanomaterials

Nanobiotechnology – nanomachines: covalent and non-covalent approaches – Molecular devices – Single molecule devices – Nanotribology and its applications – Impact of the branch of science on the society.

UNIT V: Supramolecular Chemistry

Basic concepts - Supramolecular interactions: ionic and dipolar, Hydrogen bonding, π interaction, van der Waals interaction, Hydrophobic effect.

Self assembly: Definition and basic concepts, Enthalpic and entropic considerations – Self assembly with modification: Design principles of self assembly: Symmetry interaction model – Molecular library model.

Metal directed self assembly: Racks, Ladder, Grids and Helicates – Molecular polygons – molecular triangles, molecular squares – Topological connectivity and examples for rotaxanes, catenation and knots.

Self assembling capsules: Metal directed capsules and examples for molecular scalfolding and molecular panelling – Hydrogen bonded capsules – Biological self assembly - examples only (proteins, DNA & Viruses) - Applications of supramolecules.

REFERENCE:

1. D.A. Skoog, F.J. Holler, T.A. Nieman, Thomson, Principles of Instrumental Analysis, 5th Ed. Bangalore, 2005, pp. 288 – 293.
2. D. L. Andrews, Laser in Chemistry, 3rd ed. Springer, 1997.
3. Atkins, Physical Chemistry, 7th ed. Oxford press, 2010.
4. T. Pradeep, Nano: The essentials: Understanding Nanoscience and Nanotechnology, Tata Mc Graw Hill, New Delhi, 2007.
5. Jonathan W. Steed, David R. Turner, Karl J. Wallace, Core Concepts in Supramolecular and Nanochemistry, John Wiley & Sons, 2007, pp. 1-3, 17-26, 106-113, 121-136, 139, 146, 155 – 158, 160, 163-165.

PAPER III – ADVANCED SYNTHETIC AND SPECTRAL TECHNIQUES

UNIT I: Green Chemistry

Introduction – Principles of Green Chemistry – Toxicity of chemicals in the environment – Toxic heavy metal ions – Reactions without heavy metals – Solvent less organic synthesis – Supercritical carbon dioxide and water as solvents – Ionic liquids – Reactions of solid supported catalysts – Biocatalysts – Materials for a sustainable economy – Use of Natural polymers – Polymers from renewable raw materials – Chemistry of recycling.

UNIT II: Reagents and Rearrangements

Intramolecular and Intermolecular rearrangements – Migratory aptitude of groups – Mechanism and synthetic utility of the following rearrangements: Wolf, Neber, Stevens – Cope – Hofmann – Loffler and benzidine.

Reagents and novel reactions:
Suzuki coupling – Prevost reagent – Dithianes – Phase transfer catalysts – Phosphorus and sulphur ylides.

UNIT III: Dynamic NMR spectroscopy

Introduction: Quantitative calculations – Complete line shape analysis, Coalescence temperature T_c - Rate constant k_c, Activation parameters E_A, ΔG - Intermolecular exchange process.

Applications: Rotations about C–C single bonds, $C(sp^3)$–$C(sp^3)$, $C(sp^2)$-$C(sp^3)$, $C(sp^2)$–$C(sp^2)$ bonds. Rotation about partial double bond - Inversion at nitrogen and phosphorous atoms - Ring inversion - Valence tautomerism - Keto–enol tautomerism - Intermolecular proton exchange - CIDNP technique.

Fluxional behaviour, Basic principles, Fluxional behaviour in allylic, cyclopentadienyl and cycloheptatrienyl systems.

UNIT IV: Multinuclear NMR and correlation spectroscopy

Basic principles of ^{15}N, ^{31}P and ^{19}F NMR spectroscopy – references used – chemical shifts – coupling constants. ^{15}N chemical shifts in amines, amide, urea, heterocyclic aromatic compounds, EDTA complexes – effects due to protonation and electronegative gamma substituents. Applications of ^{15}N in elucidating the stereochemistry of cis- and trans-azoxybenzene, cis- and trans- fused decahydroquinolines and tautomeric behavior of porphyrin system –Inference of ^{19}F on the ^{1}H & ^{13}C NMR spectra due to spin-spin coupling [CH_3CHFBr, $CDHF_2$] Applications of ^{31}P and ^{19}F NMR spectroscopy in elucidating the structures of some simple inorganic compounds [ClF_3, IF_5, H_2PF_3, H_3PO_2, H_3PO_3, H_3PO_4, PCl_2F_3, TiF_4L_2, $HP_2O_5^{3-}$ and meridonal and facial isomers of $Rh(PPh_3)_3Cl_3$

UNIT V: Computational Chemistry

Outline and tools of computational chemistry – potential energy surface – stationary points – Born – oppenheimer approximation – geometry optimization – Molecular mechanics – Developing a force field – force field parameterization –uses

and strengths and weakness of molecular mechanics - Basic principles of Ab-initio method & DFT methods

REFERENCE:

1. Albert S. Matlack, Introduction to Green Chemistry, second edition, CRC Press, New York, 2010.
2. Horst Friebolin, Basic One- and Two Dimensional NMR Spectroscopy, VCH, New York, 1991.
3. George C. Levy, Robert L. Litcher, Nitrogen-15 Nuclear Magnetic Resonance Spectroscopy, A Wiley-Interscience Publication, 1979.
4. J.B. Lambert, Multinuclear NMR approach, 1st edition, D. Reidel publishing Co., 1983.
5. R. S. Drago, Physical methods in Chemistry, Saunders, 1999.
6. E.A.V. Ebsworth, D.W.A Rankin and C. Craddock, Structural methods in Inorganic Chemistry, ELBS, 2nd edition, Blackwell, 1991.
7. R. M. Silverstein and F.X. Webster, Spectrometric identification of organic compounds, John Wiley, 1998.
8. Jerry March, Advanced Organic Chemistry, Reactions, Mechanism and structure, 4th edition, John-Wiley Publications, 2004.
9. J. Singh and L.D.S. Yadav, Organic synthesis, Pragati Prakasham, 2006.
10. Peter Sykes, A guide book to reaction mechanism in Organic Chemistry, Dorling Kinderslay publication, 2007.
11. Errol Liwards; Computational Chemistry, Introduction to the theory and applications of molecular and quantum mechanics: Springer publications, 2006. (pp: 1-3, 9-33, 43-57, 72-75, 159-175, 339-348, 377-378)

PAPER – IV – (1)

Coordination Chemistry, Crystal Engineering and Catalysis

UNIT I Synthesis and characteristics of coordination compounds Characterization of compounds – structure from chemical data – stoichiometry – Distinguishing non – equivalent atoms – chemical analysis and elementary physical methods – melting point, cryoscopy, elemental analysis. Preparation and Characterisation of N-2-[3-methylpyridyl-N'-phenylthiourea] transition metal complexes. Synthesis, Spectral (IR, UV-visible and Variable temperature NMR) characterization and crystal structure of (N-benzyl-N-furfuryldithiocarbamato-S-S')(thiocyanato-N)(triphenylphosphine)nickel(II) .

UNIT II Thermal analysis of Coordination Compounds

Theory, instrumentation and applications of thermogravimetric analysis (TGA) and Differential thermal analysis (DTA) – Thermal studies on metal dithiocarbamato complexes – A Review. Thermal studies of Zn(II), Cd(II) and Hg(II) complexes of some N-alkyl-N-phenyl-dithiocarbamates.

UNIT III Metal – dithiocarbamate complexes

1. Synthesis and spectral studies on Pb(II) dithiocarbamate complexes containing benzyl and fufuryl groups and their use as precursors for PbS nanoparticles.

2. Synthesis, characterization, cytotoxicity and antimicrobial studies on bis (N-fufuryl-N-(2-Phenylethyl)dithiocarbamato-S,S')zinc(II) and its nitrogen donor adducts.

3. Supramolecularly linked linear polymers of thallium(I) dithiocarbamates: Steric influence on the supramolecular interactions of methyl and ethylcyclohexyl dithiocarbamates of thallium(I)

4. Heterodinuclear ruthenium(II) bipyridyl–transition metal dithiocarbamate macrocycles for anion recognition and sensing.

5. Effect of pyridine as a ligand in precursor on morphology of CdS nanoparticles

UNIT IV Crystal Engineering

Introduction to crystal Engineering – Definition – Intermolecular interactions – Polymorphism – Multi component molecular Crystals – Co-crystal – Supramolecular retrosynthesis – The Synthon as a simplifier of crystal structures – Molecular architecture and supramolecular association in the zinc-triad 1,1-dithiolates. Steric control as a design element in crystal engineering.

UNIT V Catalysis

Catalytic processes, homogeneous and heterogeneous systems, examples, Supported catalysts, merits and demerits, Supports like organic polymers, zeolite clay materials, cellulose; Anchoring of catalysts on the supports, characterization of the catalysts (SEM, pore size determination, surface studies) Catalytic oxidation, Principles of green chemistry.

TEXT BOOKS AND REFERENCES:

1. The synthesis and characterization of Inorganic compounds, W. L. Jolly, Prentice Hall, NC, Canada 1970.

2. Physical methods in Inorganic Chemistry, R. S. Drago, W. B. Saunders Co., 1965
3. E. M. Shoukry, H. A. Bayoumi, M.M.Mostafa, Transition Met. Chem., 25, (2000) 73 – 79.
4. P.Valarmathi, S. Thirumaran, Lovely Sarmal and Rajni Kant, Spectrochim Acta,

Part A, DOI : 10.1016/j.saa.2014.03.068.
5. Quantitative analysis, R.A. Day and A.L. Underwood, Prentice-Hall, VI edition 1999.
6. Principles of Instrumental anlaysis, S. Skoog, Holler and Nieman, Saunders, 1998.
7. S. K. Sengupta and Shyam Kumar, Thermochim. Acta, 72, (1984) 349-361.
8. D.C. Onwudiwe, P.A. Ajibade, Int. J. Mol. Sci., 13 (2012) 9502-9513.
9. E.Sathiyaraj and S. Thirumaran, Spectrochim. Acta, Part A, 97 (2012) 575-581.
10. P. Jamuna Rani and S. Thirumaran, Eur. J. Med. Chem., 62 (2013) 139-147.
11. N. Alexander, K. Ramalingam and C. Rizzoli, Inorg. Chim. Acta, 365 (2011) 480-483.
12. M. D.Pratt and P. D. Beer, Tetrahedron, 60 (2004) 11227-11238.
13. N. Srinivasan and S. Thirumaran, Superlattices Microstruct., 51 (2012) 912-920.
14. Gautam R. Desiraju, J. Chem. Sci., 122 (2010) 667 – 675.
15. J. Zukerman-Schpector and E. R.T. Tiekink, Z. Kristallogr., 223 (2008) 233-234.
16. E. R. T. Tiekink, Cryst. Eng. Comm.,5 (2003) 101-113.
17. Catalysis. Principles and Applications, Editors: B. Viswanathan, S. Sivasankar and A.V. Ramaswamy, Narosa Publishing House, 2004.
18. Catalysed Oxidation of Organic Compounds: Sheldon R. A. Kochi. J. K. Metal Academic Press New York, 1981.
19. Green Chemistry, Theory and Practice: Anastas P. T, Warmer. J.C. Oxford University Press, Oxford 1998.
20. T. Punniyamurthy and Laxmidhar Rout, Coord., Chem Rev., 252 (2008) 134-154.

PAPER-IV – (2)
COMPUTATIONAL CHEMISTRY

UNIT-I

BASIS SET

Introduction; Basis-set effects: Minimal basis sets, Split valence basis sets, Polarised basis sets, Diffuse functions, High angular momentum basis set, Basis sets for Post-third row atom.

UNIT-II

MOLECULAR PROPERTIES

Computation of Geometric Parameters, Ionisation potential, Electron affinity, proton affinities and vibrational frequencies, Prediction of NMR Chemical shifts and correlation with experimental parameters, Modeling systems in solution Reaction, Field models of salvation, NBO analysis.

UNIT-III

EXCITED STATE

Configuration Interaction(CI) – single excited states, optimizations and energies, Restricted or Unrestricted computations, Frequencies, Excited state dipole moments, polarisabilities and Hyperpolarisabilities, Photochemical behaviour of some simple molecules (Butadiene, Ethylene) from computational point of view.

UNIT-IV

NON- LINEAR OPTICS

Linear optics, Non-linear optics – Second harmonic generator, NLO chromophores common NLO materials – (Inorganic, Organic semiorganic NLO materials.) Dipolemoment, polarizability, Hyperpolarizability theortical calculations and comparison with experimental parameters,.

UNIT-V

COMPUTATIONAL METHODS IN DRUG DISCOVERY

Software – List of software used in computational chemistry- Schrödinger software-Bioluminate-Homology modeling, Antibody modeling, residue scanning, cysteine mutation, protein refinement, protein-protein docking. Combiglide-Receptor grid generation, reagent preparation, combinatorial screening, combinatorial library enumeration, interactive enumeration and docking. Desmond- system builder, minimization, molecular dynamics, simulation quality analysis, simulation event analysis. Glide- Ligprep-Protein preparation-receptor glide generation-docking. Jaquar-single point energy-optimization-transition state-reaction co-ordinate-P^{ka} , Hydrogen bond, Fulki functions. Phase- Developing pharmacophore model, Building or editing hypotheses, preparing a 3D database for searching, Finding matches to a hypothesis, Running jobs. Qikprop- Running Qikprop in Normal processing mode, Running Qikprop in fast processing mode.

Case Studies:

1. Jaguar: A High-Performance Quantum Chemistry Software Program with Strengths in Life and Materials Sciences Art D. Bochevarov,*[a] Edward Harder,[a] Thomas F. Hughes,[a] et all.,**International Journal of Quantum Chemistry 2013, 113, 2110–2142**

2. Synthesis, stereochemistry, antimicrobial evaluation and QSAR studies of 2,6-diaryltetrahydropyran-4-one thiosemicarbazones.

   Umamatheswari S[1], Balaji B, Ramanathan M, Kabilan S
   Eur J Med Chem. 2011 Apr; vol.46 iss 4 p-1415-24

References:

1. A quantum theory, Oxford University Press, Oxford, 1990
2. Tripathy S.et al chem. Tech 19, 620 (1989)
3. Tripathy S.et al chem. 19, 747 (1984)
4. Chan T.V optical engineering 20, 220 (1981)
5. Prasad P. Williams D. Introduction to non-linear optical effects in molecules and polymers, John Wiley and sons 1991
6. Virtual Screening, Identification and In Vitro Testing of Novel Inhibitors of O-Acetyl-L-Serine Sulfhydrylase of Entamoeba histolytica Isha Nagpal, Isha Raj, Naidu Subbarao*, Samudrala Gourinath*
PLoS ONE 2 February 2012 | Volume 7 | Issue 2 | e30305
7. A plausible explanation for enhanced bioavailability of gpsubstrates in presence of piperine: simulation for next generation of P-gp inhibitors
Durg Vijay Singh & Madan M. Godbole & Krishna Misra
J Mol Model. 2013 Jan; Vol.19 iss.1, p-227-38.
8. Synthesis, antimicrobial evaluation and QSAR studies of novel piperidin-4-yl-5-spiro-thiadiazoline derivatives
Umamatheswari S[1], Balaji B, Ramanathan M, Kabilan S.
Bioorg Med Chem Lett. 2010 Dec 1;Vol-20 iss.23 P- 6909-14.

PAPER – IV – (3)

ORGANIC LIGHT EMITTING DIODES AND SEMI CONDUCTOR NANO MATERIALS

UNIT I: ORGANIC-LIGHT-EMITTING DIODE MATERIALS

OLEDS – basic structure – fabrication procedure – basic operation – working mechanism – design of multiple structure – molecular materials for OLED'$_S$ – HTL, ET, emitter, dopant material.

Reference:

1. Survey, Organic Light Emitting Devices, Edited by: Joseph Shinar, Ames Laboratory-USDOE & Department of Physics and Astronomy, Lowa State University, Ames, IA, 2012.

UNIT II: DOPED OLEDS

1. Physicochemical Studies Of Green Phosphorescent Light-Emitting Materials from Cyclometalated Heteroleptic Iridium (III) Complexes, J. Jayabharathi, V. Thanikachalam, N. Srinivasan, M. Venkatesh Perumal, Spectrochim. Acta A. 2011, 79, 338-347.
2. Tuning the emission and morphology of cyclometalated iridium complexes and their applications to organic light-emitting diodes, Fang-Iy Wu, Huei-Jen Su, Ching-Fong Shu, Liyang Luo, Wei-Guang Diau, Chien-Hong Cheng, Jiun-Pey Duan and Gene-Hsiang Lee, **J. Mater. Chem.**, 2005, **15**, 1035-1042.

UNIT III: CURRENT RESEARCH ON OLEDS

1. J. Jayabharathi, P. Ramanathan, V. Thanikachalam, Synthesis and optical properties of phenanthrimidazole derivatives for organic electroluminescent devices, *New J. Chem.,* 2015, 39 (1), 142-154.
2. J. JayabharathI, P. Ramanathan, C. Karunakaran, V. Thanikachalam, Fused methoxynaphthyl phenanthrimidazole semiconductors as functional layer in high efficient OLEDs, *J. Fluoresc.,* 26 (2016), 307–316,

UNIT IV: NON-DOPED OLEDS

1. J.Jayabharathi, A. Prabhakaran, V.Thanikachalam, P. Jeeva, Efficient non-doped blue emitting devices based on bis(phenanthrimidazolyl)biphenyl derivatives, *ACS.Ind. Eng. Chem. Res.,* 2016, 55 (29), 8087–8095.
2. J. Jayabharathi**,** A. Prabhakaran, V. Thanikachalam, M. Sundharesan, Highly efficient non-doped blue electroluminescent materials for organic light-emitting devices, *RSC Adv.*, 2016, 6, 62208–62217.

UNIT V: HyLEDs-Hybrid Light Emitting Diodes

1. Hybrid organic-inorganic light emitting diodes: Effect of Ag-doped ZnO, J. Jayabharathi, A. Prabhakaran, V.Thanikachalam, M. Sundharesan, *J. Photochem. Photobiol. A. C.,* 2016, 325, 88-96.

   Organic and hybrid organic-inorganic light emitting devices.

PAPER-IV-4
PHOTOCHEMISTRY

UNIT I
CURRENT TOPICS IN PHOTOCHEMISTRY

The laws of photo chemistry – Quantum Efficiency and its experimental determination – Jablonski diagram – Fluorescence, phosphorescence, Chemiluminescence- Nature of chemiluminescence reactions photosensitization – photosynthesis - Lasers – Types of Lasers- Gas lasers, metal vapour laser. Semiconductor Laser- Types, characteristics and applications. – Photochemical reactions of metal complexes.

UNIT II
PHOTOCATALYTIC DEGRADATION OF POLLUTANTS IN WATER

Role of Photonic Excitation, Electron Transfer, and Adsorption, Photocatalytic Character of a Reaction, Chemical Kinetics and Information on reaction mechanisms, Semiconductor photocatalysis-Mechanisms of Semiconductor Photocatalysis, Metal Oxide Semiconductors(TiO_2,ZnO etc.,) Metal ion dopant and Photoreactivity. In-depth Treatment of the Technique, Roles of O_2, Effects of H_2O_2 and O_3, Fenton reagent, Fenton Reaction - mechanisms and kinetics, Scavengers, Haber–Weiss Reaction, Advanced Oxidation Process, Photo–Fenton, Heterogenous photo–Fenton. Other transition metal ions participating Fenton-type cycles, hydroxyl radical reactions with organic Compounds, Typical in situ Applications

UNIT III
PHOTOCATALYSIS FOR SOLAR ENERGY CONVERSION

Solar photocatalysis, solar Photocatalytic Process, Quantum Yield, Catalyst Related Losses, Carrier thermalization, Charge separation - Active charge separation, passive charge separation, Mediated charge separation, Surface-related losses, Photoelectrochemical Cells, Crystal structure and activity, Visible light sensitization , Zeolite based Quantum dots relevents to solar energy applications, Photocatalytic water spilitting, The Hydrogen evolution reaction: Water reduction photocatalysis - improved Niobate Nanoscroll Photocatalysts.

UNIT IV
PREPARATIVE TECHNIQUES

General features of a zeolites and their cavities – Synthesis of Zeolite – $(Na_x(AlO_2)_x(sio_2)_y)_mH_2O$-preparation of thin films – chemical vapour deposition, Hydrothermal technique, zone melting – Types of Nanomaterials – Synthesis of Nanomaterials – Sol-gel method – Thermal decomposition method, Sonochemical method, Physical vapour deposition method.

UNIT V
TECHNIQUES FOR CHARACTERIZATION OF NANOMATERIALS

Scanning electron microscopy (SEM), Field emission scanning electron microscopy (FE-SEM), Transmission electron microscopy (TEM), High resolution Transmission electron microscopy (HR-TEM) ,X-ray diffraction (XRD), Photo Luminescence (PL), Atomic force microscopy (AFM), Scanning Probe microscopy(SPM), UV-Diffused reflectance

spectroscopy (UV-DRS), Energy dispersive spectrum (EDS), Elemental Mapping, Brunauer-Emmett-Teller(BET) surface area measurements and particle size analysis.

References:

1. K.K. Rohatgi Muherjee, Fundamental of photochemistry, M.C. Graw Willey Eastern, 1994 publication.
2. Nicholas, J. Jurro, Modern molecular photochemistry, The Benjamin publishing company, California, 1978.
3. Ferraudi G.L, Elements of inorganic photochemistry, Wiley Eastern, Ebsworth E.A.V. Rankine and S.Craddock, ELBS, 1991.
4. Coxon and Halton, Organic photochemistry, Cambridge University Press,
5. Deputy c, Hand O.S.chapman, Elements of organic photochemistry, Prentice-Hall, 1975.
6. Skoog. S, Holker and Nieman, "Principles of instrumental Analysis", Saunders, 1998.
7. Pradeep. T, "Nano", The essentials; understanding Nano science and Nanotechnology, Tata Mc Graw Hill, New Delhi 2007.
8. Mick Wilson, Kamali Kannangara, GeofR Smith, Michella Simmons, Burkhard Raguse, Nano Technology Overseas Press, 2005.
9. Shah. M. A, Tokeer Ahmad Principles of Nanoscience and Nanotechnology, Alpha Science Intl Ld; 1 ed, 2010.
10. Gabriele Centi, Rutger A.van Santen Catalysis for Renewables: From Feedstock to Energy Production Wiley-VCH Verlag GmbH & Co.KGaA, 2007
11. Klabunde K. J and Richards R.M, Nanoscale materials in Chemistry, A john Wiley & sons INC publications, Second ed. 2009
12. Matthew A. Tarr, Chemical Degradation Methods for Wastes and Pollutants. Marceld ekkerin, C Publishers, USA 2003
13. Townsend TK, Inorganic metal oxide nanocrystal photocatalysts for solar fuel generation from water springer publication, 2014
14. Vincenzo Balzani, Alberto Juris, Photochemistry and Photophysics of Ru(11) polylpyridine complexes in the Bologna group. From early studies to recent developments, Coodinatiom chemistry reviews 211 (2001) 97-115.

PAPER- IV – (5)
CRYSTALLIZATION AND SURFACE CHEMISTRY

UNIT I: Crystalline state

Liquid crystals – isotropic and anisotropic liquids – crystalline solids – simple contact goniometer – reflecting goniometer –crystal symmetry – crystal systems – Miller indices crystal symmetry – crystal systems – Space lattices – crystal habit – composite crystals and twins – parallel growth – interpenetrant twins.

UNIT II: Nucleation

Introduction – primary nucleation – homogeneous nucleation – measurement Techniques – spinodal decomposition – heterogeneous nucleation – secondary nucleation – contact nucleation – seeding, metastable zone widths–effect of impurities –latent periods – Ostwald's rule of stages.

UNIT III: Crystal Growth

Crystal growth theories – surface energy theories – adsorption layer theories – diffusion-Reaction theories. Birth and spread models- crystal surface structure – crystallization from melts –growth and nucleation rates- effect of temperature – effect of crystal size –growth rate measurements –low temperature solution growth – high temperature solution growth, growth in gels – temperature lowering methods – hydrothermal growth – growth from the melt– growth from vapours.

UNIT IV: X-ray Diffraction by Polycrystalline Materials.

Kinematic and geometric theories of X-ray diffraction – scattering by an atom, scattering by a free electron – coherent Scattering – the Thomson formula, incoherent scattering – compton scattering – scattering by a bound electron – scattering by a multi-electron atom – diffraction by an ideal crystal –direct lattice – Reciprocal lattice – instrumentation used for X-ray diffraction – different elements of a diffractometer– X-ray source, crookes tubes, coolidge tubes, high intensity tubes, Synchrotron radiation – filters and mono chromator crystals – detectors- photographic film – gas detectors, solid detectors. Data processing – extraction information – Peak profile.

UNIT V: Surface chemistry

Self assembly – colloids – structure & stability – micelles – formation – micellar catalysis – membrane formation – surface films – the thermodynamics of surface layers – gel – surfactant – emulsification – stability of emulsions - electrodialysis – solubilisation – gels – preparation – importance.

REFERENCES:

1. J.W.Mullin. Crystallization, Fourth edition, University College London 2001.
2. Rene Guinebretiere. X-ray Diffraction by Polycrystalline Materials, Published in Great Britain and the United States in 2007 by ISTE Ltd.
3. Advanced Physical Chemistry – By Prof. Gurdeep Raj. Goel Publishing House. A unit of Krishna Praskashan Media (P) ltd., 1978.
4. Physical Chemistry, PETER ATKINS, 8th edition, International student edition, 2006.

PAPER IV – (6): ORGANIC SYNTHESIS, SPECTROSCOPY AND MEDICINAL CHEMISTRY

Unit-I: NAMING REACTIONS AND NOVEL ORGANIC TRANSFORMATIONS:
Heck reaction, Negshi coupling, Suzuki coupling, alkene metathesis, ring closing alkene metathesis, Ene reaction, Diels Alder reaction, Claisen rearrangement, Cope rearrrangement, 1,3- Dipolar cycloaddition, Sigmatropic reactions(1,5), (1,7), (3,3), Wagner-Meerwein reactions, Tiffeneau- Demjanov rearrangement, Chiral auxillaries and their applications.

Unit-II: REAGENTS IN ORGANIC SYNTHESIS:
Use of the following reagents in organic synthesis and functional group transformations; 1,3-propanedithiol, m-chloroperbenzoic acid(m-CPBA),lithium aluminum hydride, sodium borohydride, DIABAL-H and solvent effect, Osmium tetraoxide and potassium permanganate, Diazomethane, sulphur and phosphorus ylides. .

UNIT-III: SPECTROSCOPY
IR Spectroscopy-vibrational frequencies and factors affecting them-identification of functional groups-intra and intermolecular hydrogen bonding. Principles of ^{1}H-NMR – chemical shift and coupling constants-factors influencing proton chemical shifts and vicinal coupling constants. ^{13}C NMR- proton decoupled and off-resonance ^{13}C NMR spectra-factors affecting ^{13}C chemical shifts.
Principles of two dimensional correlated NMR spectroscopy, ^{1}H-^{13}C COSY, ^{1}H-^{1}H COSY, Two-dimensional relayed NMR spectroscopy, H relayed (H, C) COSY, H relayed (H, H) COSY experiments. Two-dimensional exchange NMR-NOESY. Total correlation spectroscopy, Two-dimensional inadequate experiment.

UNIT-IV: MEDICINAL CHEMISTRY
Development of new drugs, procedures followed in drug design, concepts of pro drugs and soft drugs, structure-activity relationship (SAR), factors affecting bioactivity, resonance, inductive effect, isosterism, bio-isosterism, stereo specific aspects of drug action. Theories of drug activities: occupancy theory, rate theory, induced fit theory, quantitative structure activity relationship. Method used in QSAR studies linear free energy related (LFER) – Hansch- mixed approach – Free Wilson theory. Elementary treatment of drug receptor interactions.
Protein binding- forces involved in drug-protein interaction, factors affecting drug-protein binding, mathematical derivations, methods employed to detect the drug-protein interactions.

UNIT-V: APPLIED MICROBIOLOGY
Experimental techniques in Antioxidant studies Antifungal studies Antibacterial studies Anticancer studies

REFERENCE:

1. Advanced organic chemistry, A. Carey and Sundberg, 5th edition.part1&2
2. Reagents in organic chemistry by House.
3. Horst Friebolin, Basic One and Two Dimensional NMR Spectroscopy, VCH, New York, 1991.
4. R.M. Silverstein and F.X. Webster, Spectrometric identification of organic compounds, John wiley, 1998.
5. S.S. Kadam, K.R. Mahadik, K.G. Bothara, Principles of medicinal chemistry, Volume-I and II, Nirali Prakashan, 2005.

6. Micheal J.Lebuffe, Burton E.Piere, Microbilogy; Laboratory theory and application, Morton publishing company, 2008.
7. Kathleen Park Talaro, Foundations in Microbiology Basic principles, 6th Edition, McGraw Hill international,2007.

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PAPER- IV – (7)
HYBRID MATERIALS

UNIT – I

Perovskites - synthesis - structure – structure predictions – dissociation to garnets – dielectric constant discontinuity - size effects – changes in composition – Jahn-Teller effects – Magnetism – Electronic correlations – Cuprates – Manganites – Synthetic minerals – synthetic Perovskites – octahedral tilting – cation deficient – synthetic spinels.

UNIT – II

Layered oxides - Manganese oxide – Structures of porous manganese oxide crystals - Synthesis of tunnel and layered manganese oxides - Melting salt flux process - Redox precipitation process Sol–gel process - Hydrothermal process - Extraction/insertion reactions with metal ions - Hollandite-type manganese oxide - Todorokite-type manganese oxide - Birnessite-type manganese oxide - Ion-sieve and molecular-sieve properties - Ion-sieve properties – Molecular sieve properties - Electrochemical extraction / insertion reactions - Applications as adsorbents and catalysts

UNIT - III

Layered iodides – importance of PbI_2 - polytypism of lead iodide - structure of PbI_2 - The 2H, 4H, 6H, and 6R polytypes of PbI_2 - Geometry of the near-octahedral structure of the $[PbI_6]^{4-}$ - Ion exchange and intercalation – Redox intercalation/deintercalation – Acid leaching Intercalation in lead iodide – Packing in lead iodide – intercalation of hydrazine in lead iodide – Effects of intercalation – Band edge shift on intercalation.

UNIT - IV

Hybrid materials – organic-inorganic hybrid materials – hydrothermal synthesis – Role of organic component – organodiamine coordination polymers – Polymers involving 4,4'-bipyridine - Two and three dimensional: One– and two- dimensional polymers with tethered amines - Three dimensional polymers with tethered amines –Polymers from three connected ligands – Polymers with hexamethylenetetramine as linker ligand – Prelude to oxide - copper sulfate- organodiamine system .

UNIT - V

Synthesis and crystal chemistry of hybrid perovskites – ABX_3 (where A = organic cation, , B = Ge, Sn, Pb, X = halide) – $(CH_3NH_3)PbX_3$, $(CH_3NH_3)SnX_3$, $HC(NH_2)_2SnI_3$, $HC(NH_2)_2PbI_3$ - Thermal analysis – optical properties – Seebeck coefficient – Carrier concentration – solar cell applications – Chemistry behind solar cell – Current conversion efficiency.

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