

M.Phil. CHEMISTRY SYLLABUS

(For the candidates admitted from the academic year 2019 – 2020 onwards)

(Under Choice Based Credit System)



PG Department of Chemistry

Nehru Memorial College (Autonomous),

(Affiliated by Bharathidasan University)

(Accredited with 'A' grade by NAAC)

Puthanampatti – 621 007

Eligibility: M.Sc. Chemistry

PROGRAMME OBJECTIVES:

- To impart advance knowledge of chemistry in different subjects which are required to understanding philosophy of chemistry.
- To train post graduates capable of undertaking higher level chemical research.
- To produce skilled postgraduates who can act in the increasingly wide research area of chemistry.
- To practice innovative teaching methods to communicate clearly and effectively, orally and in writing.
- This programme can also be extended to PhD studies by the addition of one year's worth of research.

PROGRAMME STRUCTURE

NEHRU MEMORIAL COLLEGE (AUTONOMOUS), PUTHANAMPATTI – 7

M.Phil. CHEMISTRY (FT/PT) Programme

(For the candidates admitted from the academic year 2019 – 2020 onwards)

COURSE STRUCTURE

SEMESTER – I	COURSE TITLE	MARKS			CREDITS
		IA	UE	TOT	
COURSE – I	Research Methodology	25	75	100	4
COURSE – II	Physical Methods in Chemistry	25	75	100	4
COURSE – III	Teaching and Learning Skills	25	75	100	4
COURSE – IV	Elective – (Any one)	25	75	100	4
	Elective Papers 1. Chemical kinetics 2. Phytochemistry and Natural products 3. Advanced Inorganic chemistry 4. Co-ordination Chemistry and Spectroscopy 5. Advanced Organic and medicinal Chemistry				

SEMESTER – II

Dissertation and Viva – Voce	Viva Voce – 50 Marks Dissertation – 150 Marks	200(150+50)	8
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Course code & Title	PAPER – I: RESEARCH METHODOLOGY		
M.Phil. Chemistry	Semester -I	Credits: 4	Hrs/Wk: 6
Cognitive Level	K1 Acquire K2 Understand K3 Apply K4 Evaluate K5 Analyze		
Course Objectives	The course aim <ul style="list-style-type: none"> • Develop skills of literature survey, Research proposal and preparation records • Appreciate the role of statistical tools for research • Acquire the knowledge of computer in chemistry and separation techniques • To get knowledge in laboratory practices and safety • To familiarize the project management 		

UNIT – I - RESEARCH METHODOLOGY:

Meaning, Scope, Primary sources of literature survey, Journals, patents etc., secondary sources of literature survey, Books, Reference books, Text books, listing of letters. **Research problem:** meaning of research problems, sources of research problems, criteria / characteristics of a good research problem, errors in selecting a research problem and research ethics. **Hypothesis:** Meaning, types of hypothesis. **Developing a Research Proposal:** Format of research proposal, individual research proposal and institutional proposal. **Research Report:** Format of the research report, style of writing the report, references and bibliography **Preparation of Records** – Manuscripts – Research Paper formats in Indian J.Indian Chem. Soc., Tetrahedron, etc.,

UNIT – II – STATISTICAL TOOLS OF RESEARCH

Types of Error – Accuracy, precision, Significant figures-Tests for accuracy of results-positive and negative deviation from accuracy. Distributions- Binomial, Gaussian, etc., The normal distribution of random errors-mean value-Variance-Standard deviation-reliability interval – t-test-F-test. Regression-standard deviation-Correlation coefficient-Multiple linear regression-Observation. Inference-Hypothesis generation-Testing of Hypothesis. Evolving and modifying Rules & Theories.

UNIT – III – COMPUTER APPLICATIONS IN CHEMISTRY

Introduction to computers – history of development of computers. Main frame, mini, micro and super computer systems. Computer hard ware CPU, input, output devices, auxiliary storage devices, interpreter, compiler, machine language, assembly language, high level languages. Operating systems-MS DOS, windows, UNIX. Languages – C Language & programming – constants, variable functions– Logical & arithmetic statements. Simple programming examples from chemistry Temperature conversion, C_v of solids(C_v at $T < 30\text{ K}$ and at $T > 30\text{ K}$), Activity coefficient of Electrolytes, Rate constants of I & II order reactions, Calculation of Arrhenius parameters. Introductory Operatives – Package, MS word, MS Excel, MS power Point – preparing scientific manuscripts.

UNIT - IV – GOOD LABORATORY PRACTICES AND SAFETY

Introduction: History, definition, principles, Good laboratory practices (GLP) training: Resources, Rules, characterization, Documentation, quality assurance. **Facilities:**building and equipment, personal, GLP and FDA, European Union, non-member countries. Stepwise implementation of GLP and compliance monitoring.

Safe working procedure and protective environment, protective apparel, emergency procedure and first aid, laboratory ventilation, safe storage and use of hazardous chemicals, procedures for working with substances that pose hazards, flammable or explosive hazards, procedures for working with gases at pressure above or below atmospheric – safe storage and disposal of waste chemicals, recovery, recycling and reuse of laboratory chemicals, procedure for laboratory disposal of explosives, identification, verification and segregation of laboratory waste, disposal of chemicals in the sanitary sewer system, in incineration and transportation of hazardous chemicals.

UNIT- V: PROJECT MANAGEMENT

Need for project management, project management approaches, project development stages, work breakdown structures.

Time, cost quality and risk management, tools and techniques for project management, cost estimation and budgeting, monitoring controlling and closure, continual improvement.

Text Books

1. Research Methodology. Methods and Techniques : C. R. Kothari,
2. Tests, Measurements and Research Methods in Behavioural Sciences : A. K.Singh
3. March J, 1996, "Advanced Organic Chemistry Reactions, Mechanisms and Structure." 5th ed, New York, Wiley.
4. D.B.Hibbert and J. J. Googling, Data Analysis for Chemistry, Oxford University Press, 2006.
5. J. Topping, Errors of Observation and Their Treatment, Fourth Edn., Chapman Hall. London, 1984.
6. S.C. Gupta, Fundamentals of Statistics, Sixth Edn.,Himalaya Publ. House, Delhi, 2006.
7. H. E. Solbers, Inaccuracies in Computer Calculation of Standard Deviation, Anal. Chem.. 55, 1611 (1983).
8. P.M. Wanek et al., Inaccracies in the Calculation of Standard Deviation with Electronic Calculators, Anal. Chem. 54, 1877 (1982).
9. A. M. Cogill and L.R. Gardson, The ACS Style Guide – Effective Communication of Scientific information, 3rdEdn., Oxford University Press, 2006.
10. H. Bell and J. Trimbur, A short Guide to Writing about Chemistry, 2ndEdn, Longman, 2001.
11. Handbook Good Laboratory Practice (GLP) Quality Practices for Regulated Non-Clinical, Research and Development.
12. . Good Laboratory Practice Standards: Applications for Field and Laboratory Studies (ACS Professional Reference Book) by Willa Y. Gamer, Maureen S. Barge, and James,.P
13. Chemical safety matters – IUPAC – IPCS, Cambridge Univ. Press, 1992.
14. James P. Lewis, Fundamentals of Project Management. 3rd Edition, AMACOM, 2006.

References

1. <http://www.Virtualref.com/govdocs/s189.htm>
2. <http://www.inflibnet.ac.in>
3. <http://www.springerlink.com>
4. <http://rsc.org>
5. <http://www.pubs.acs.org>
6. <http://dspace.org>
7. <http://dspace.bdu.ac.in>
8. B.S. Furniss, A.J. Hannaford, P. W. G. Smith, A.R. Tatchell, Vogel's Text Book of Practical Organic chemistry, 5th Edition, Pearson, New Delhi, 1989.
9. V. K. Srinivasan and K. K. Sreemivastave, Introduction to Chromatography, S.Chand & Co., New Delhi, 2nd edition, 1981.
10. C. H. Hamann, A. Hammett and W. Vilelstick, Electrochemistry, Wiley – VCH, 1998.
11. A.J. Bard and L.F. Faulkner, Electrochemical methods – Fundamentals and Applications, 2nd Edn., Wiley-VCH, 1998.
12. A. C. Fisher, Electrode Dynamics, Oxford University Press, 1996.
13. J. Koryta and K. Stulik, Ion-Selective Electrodes, Cambridge University Press 1983.
14. Christopher.M.A and Ana Maria Oliveira Brett, "Electroanalysis" Oxford University Press, Oxford, 1998.
15. Daniel C. Harris, "Quantitative Chemical Analysis", Third Edn., W.H. Freeman and Company New York, 1996.
16. A. J. Bard L.F. Faulkner, Electro Chemical methods – Fundamentals and Applications, Second Edn., Wiley-VCH, 1998.
17. Joseph Wang, "analytical electrochemistry", Second Edn., Wiley-VCH, 2001.

Course outcomes:

- The scholars will know the different routes to design a research problem
- General terminology including various methods for the research shall be the outcome of the course.
- To improve the numerical aptitude and computational knowledge in the basic of collection and presentation of data.
- The scholars will acquire knowledge of safe laboratory practices by handling laboratory glassware, equipment, and chemical reagents.

Course code & Title	PAPER – II: Advanced Physical Methods in Chemistry		
M.Phil. Chemistry	Semester -I	Credits: 4	Hrs/Wk: 6
Cognitive Level	K1 Acquire K2 Understand K3 Apply K4 Evaluate K5 Analyze		
Course Objectives	The course aim <ul style="list-style-type: none"> • Develop skills of instruments and apply them in research • Appreciate the role of spectroscopy in research • To familiarize in EPR spectroscopy in research • To get knowledge in XRD studies • Acquire the knowledge of spectroscopy and Nano chemistry 		

UNIT – I

UV Visible spectroscopy – Instrumentation. Microstates- Term symbols and energy levels for $d^1 - d^9$ ions in cubic and square fields. Intensity of bands - group theoretical approach to selection rules - effect of distortion and spin orbit coupling on spectra - Evaluation of $10 Dq$ and β values for octahedral complexes of cobalt and nickel. Application to simple coordination compounds. Applications to organic compounds and calculation of λ_{max} - charge transfer spectra.

IR and Raman spectroscopy – Instrumentation. Combined uses of IR and Raman spectroscopy in structural elucidation of simple molecules like N_2O , ClF_3 , NO_3^- , ClO_4^- . Predicting IR bands for simple organic molecules - effect of coordination on ligand vibrations - uses of group vibrations in the structural elucidation of metal complexes of urea, thiourea, cyanide, thiocyanate, nitrate, sulphate and dimethyl sulfoxide. Effect of isotopic substitution on the vibrational spectra of metal carbonyls with reference to the nature of bonding, geometry and number of C-O stretching vibrations (group theoretical treatment). Applications of Raman Spectroscopy. Photo electron spectroscopy - Principle - Auger electron spectroscopy - electron spectra in chemical analysis.

UNIT – II – ADVANCED RESONANCE SPECTROSCOPY

NMR of paramagnetic molecules- isotropic shifts contact and pseudo contact interactions - lanthanide shift reagent. Characteristics of quadrupolar nucleus - effect of field gradient and magnetic field upon quadrupolar energy levels - NMR transitions applications – Basic principles and applications of NQR.

^1H NMR: Long-range coupling – Homotopic, enantiotopic and diastereotopic systems – Conformationally mobile, open chain systems. Virtual coupling – Coupling of proton to fluorine, phosphorous. Nuclear Overhauser effect.

^{13}C NMR: Off resonance decoupling – Coupling of carbon to deuterium, fluorine, phosphorus – DEPT – Application of proton and carbon data in identifying small organic compounds. 2D NMR: Principles of 2D NMR spectroscopy: $^1\text{H} - ^1\text{H}$ COSY, $^1\text{H} - ^{13}\text{C}$ COSY, HMBC and HSQC.

UNIT – III

EPR spectroscopy - Factors affecting the magnitudes of g and A tensors in metal species. Zero field splitting and Kramer's degeneracy- spectra of V(II), Mn(II), Fe(II), Co(II), Ni(II) and Cu(II) complexes- applications of EPR to few biological molecules containing Cu(II), Fe(II) and Fe(III) ions - spin densities and McConnell relationship. Applications of EPR to some simple systems such as CH_3 , p-benzoquinone. Xe^{2+} .

Mossbauer spectroscopy - Isomer shifts - magnetic interactions - Mossbauer emission spectroscopy - application to iron and tin compounds.

Mass spectrometry - Instrumentation - resolution, EI and CI methods - base peak, isotopic peaks, metastable peak, parent peak, determination and use of molecular formula, recognition of molecular ion peak - FAB Fragmentation - general rules - pattern of fragmentation for various classes of compounds, McLafferty rearrangement, Importance of metastable peaks.

UNIT IV

Diffraction Methods - Crystal symmetry - combination of symmetry elements – crystal classes - screw axis and glide planes - space group - crystal axes - crystal systems, unit cell, Bravais lattices, asymmetric unit - space group - Equivalent positions- relationship between molecular symmetry and crystallographic symmetry - basic concepts and examples.

X - Ray diffraction - The concept of reciprocal lattice and its applications - X-ray diffraction by single crystals - structure factor - determination of space group by symmetric phase problem in structure analysis - heavy atom method - Fourier synthesis - refinement of structure. Neutron diffraction - Magnetic scattering - applications and comparison with X-ray diffraction. Electron diffraction - Basic principles and application to simple molecules such as XeF₆, Be(BH₄)₂, Ferrocene, Cr(II)acetate.

UNIT –V –NANO CHEMISTRY

Importance and necessity for nanomaterials – Different types of nanomaterials – nanotubes, nanowires, nanorods, nanofibres and nanoflowers of polymers, semiconductors, metals and alloys – nanocrystalline materials – nanoporous materials – nanofilms. Synthesis of Nanomaterials: Wet processes – colloidal chemical method, hydrothermal method, sol-gel method.

Techniques in Nanochemistry

Techniques for Characterisation of nanoscale materials (Basic aspects): Atomic force microscopy (AFM)-Transmission electron microscopy (TEM)-Resolution and scanning transition electron microscopy (STEM) Scanning Tunneling Microscopy (STM) Scanning nearfield optical microscopy (SNOM) and surface plasmon spectroscopy.

Text Books

1. Huheey JE, Keiter EA and Keiter RA, 2000, Inorganic Chemistry, Principles of Structure and Reactivity, 4th edition, New Delhi, Pearson Education (Asia).
2. Silverstein RM and Webster FX, 2003, Spectrometric Identification of Organic Compounds, 6th edition, New York, John-Wiley and Sons Inc.
3. Kalsi PS, 1990, Stereochemistry Conformation and Mechanism, 4th edition, New Delhi, New Age International Publishers.
4. Straughan BP and Walker S, 1976, Spectroscopy vol: 1-3, London, Chapman and Hall.
5. Drago RS, 1980, Physical Methods in Chemistry, New Delhi, W. B. Saunders.

REFERENCES:

1. Acc. Chem. Res. July 2005.
2. Bengt Nolfing, 'Methods in Modern Physics', Springer, 2004.
3. T. Pradeep, Nano: The Essentials, McGraw-Hill Edn. New Delhi, 2007.
4. P.M. Silverstein, F.X. Wester, Spectroscopic Identification of Organic Compounds. 6th Ed., Wiley 1998.
5. W. Kemp, Organic Spectroscopy, 3rd Ed., MacMillan, 1994.

6. H. Gunther, NMR spectroscopy, Basic principles, concepts and application in chemistry, John Wiley & Sons, 2nd Ed., 1995.
7. R. S. Drago, Physical Methods in Chemistry, Saunders, 1977.
8. J. A. Weil, ZJ. R. Boldton and J. E. Wertz, Electro Paramagnetic Resonance: Elementary Theory and Practical Applications, John Wiley and Sons, 1994.
9. Nanotechnology – Basic Science and Emerging Technologies, MichWilson, KamaliKannagari, Geoff Smith, 2005, overseas press India private Ltd.,
10. K.L.Choy, Process principles and applications of novel and costeffective ESAVD based methods, Scientific Publishing, Singapore, 2002.
11. A. Jones and M.Mitchell, Nanotecnology-Commercial Opportunity, Evolution Capital Ltd., London, 2001.
12. C.N.R. Rao, A. Muller and A.K. Cheetham(Eds), The Chemistry of Nanometrials Vol.I& Vol. II., Wiley-VCH, 2004.

Course outcomes:

- Different analytical tools for the characterization of materials can be very well understood by the scholars.
- The scholars able to predict the concepts and applications of NMR, ESR and mass spectroscopy.
- The scholars will understand the importance of potentiometry and electro analytical techniques.
- The scholars will be able to articulate the importance of fluorescence spectroscopy.

Course code & Title	COURSE - III - Teaching and Learning Skills		
M.Phil. Chemistry	Semester -I	Credits: 4	Hrs/Wk: 6
Cognitive Level	K1 Acquire K2 Understand K3 Apply K4 Evaluate K5 Analyze		
Course Objectives	The course aim <ul style="list-style-type: none"> • Acquaint different parts of computer system and their functions. • Understand the operations and use of computers and common Accessories. • Develop skills of ICT and apply them in teaching learning context and Research. • Acquire the knowledge of communication skill with special reference to its elements, types, development and styles. • Understand the terms communication Technology and Computer mediated 		

Course Objectives :

teaching and develop multimedia /e- content in their respective subject.

- Understand the communication process through the web.
- Acquire the knowledge of Instructional Technology and its Applications.
- Develop different teaching skills for putting the content across to targeted audience.

Unit I: Computer Application Skills

Information and Communication Technology (ICT): Definition, Meaning, Features, Trends – Integration of ICT in teaching and learning – ICT applications: Using word processors, Spread sheets, Power point slides in the classroom – ICT for Research: On-line journals, e-books, Courseware, Tutorials, Technical reports, Theses and Dissertations-- **ICT for Professional**

Development: Concept of professional development; institutional efforts for competency building; individual learning for professional development using professional networks, OERs, technology for action research, etc.

Unit II : Communications Skills

Communication: Definitions – Elements of Communication: Sender, Message, Channel, Receiver, Feedback and Noise – Types of Communication: Spoken, and Written; Non-verbal communication – Intrapersonal, interpersonal, Group and Mass communication – Barriers to communication: Mechanical, Physical, Linguistic & Cultural – Skills of communication: Listening, Speaking, Reading and Writing – Methods of developing fluency in oral and written communication – Style, Diction and Vocabulary – Classroom communication and dynamics.

Unit III : Pedagogy

Instructional Technology: Definition, Objectives and Types – Difference between Teaching and Instruction – Lecture Technique: Steps, Planning of a Lecture, Delivery of a Lecture – Narration in tune with the nature of different disciplines – Lecture with power point presentation - Versatility of Lecture technique – Demonstration: Characteristics, Principles, planning Implementation and Evaluation – Teaching-learning Techniques: Team Teaching, Group discussion, Seminar, Workshop, Symposium and Panel Discussion.

Unit IV: E- Learning, Technology Integration and Academic Resources in

India

Concept and types of e-learning (synchronous and asynchronous instructional delivery and means), m-learning (mobile apps); blended learning; flipped learning; E-learning tools (like LMS; software's for word processing, making presentations, online editing, etc.); subject specific tools for e-learning; awareness of e-learning standards- Concept of technology integration in teaching- learning processes; frameworks guiding technology integration (like TPACK; SAMR); Technology Integration Matrix- Academic Resources in India: MOOC, NMEICT; NPTEL; e-pathshala; SWAYAM, SWAYAM Prabha, National academic depository, National Digital Library; e-Sodh Sindhu; virtual labs; eYantra, Talk to a teacher, MOODLE, mobile apps, etc.

Unit V : Skills of Teaching and Technology based assessment

Teaching skills: Definition, Meaning and Nature- Types of Teaching Skills: Skill of Set Induction, Skill of Stimulus Variation, Skill of Explaining, Skill of Probing Questions, Skill of Black Board Writing and Skill of Closure – Integration of Teaching Skills – Evaluation of Teaching Skills- **Technology for Assessment:** Concept of assessment and paradigm shift in assessment; role of technology in assessment ‘for’ learning; tools for self & peer assessment (recording devices; erubrics, etc.); online assessment (open source software’s; e-portfolio; quizmakers; e- rubrics; survey tools); technology for assessment of collaborative learning like blogs, discussion forums; learning analytics.

References

1. Bela Rani Sharma (2007), Curriculum Reforms and Teaching Methods, Sarup and sons, New Delhi
2. Brandon Hall , E-learning, A research note by Namahn, found in: [www.namahn.com/resources/ .../note-e-learning.pdf](http://www.namahn.com/resources/.../note-e-learning.pdf), Retrieved on 05/08/2011
3. Don Skinner (2005), Teacher Training, Edinburgh University Press Ltd., Edinburgh
4. Information and Communication Technology in Education: A Curriculum for schools and programmed of Teacher Development, Jonathan Anderson and Tom Van Weert, UNESCO, 2002.
5. Jereb, E., & Šmitek, B. (2006). Applying multimedia instruction in e-learning. Innovations in Education & Teaching International, 43(1), 15-27.
6. Kumar, K.L. (2008) Educational Technology, New Age International Publishers, New Delhi.
7. Learning Management system: https://en.wikipedia.org/wiki/Learning_management_system , Retrieved on 05/01/2016
8. Mangal, S.K (2002) Essential of Teaching – Learning and Information Technology, Tandon Publications, Ludhiana.
9. Michael, D and William (2000), Integrating Technology into Teaching and Learning: Concepts and Applications, Prentice Hall, New york.

10. Pandey,S.K (2005) Teaching communication, Commonwealth Publishers, New Delhi.

11. Ram Babu,AabdDandapani,S (2006), Microteaching (Vol.1 & 2), Neelkamal Publications, Hyderabad.

12. Singh,V.K and Sudarshan K.N. (1996), Computer Education, Discovery Publishing Company, New York.

13. Sharma,R.A., (2006) Fundamentals of Educational Technology, Surya Publications,Meerut

14. Vanaja,M and Rajasekar,S (2006), Computer Education, Neelkamal Publications, Hyderabad.

Course Outcomes

- After completing the course, the students will:
- Develop skills of ICT and apply them in Teaching Learning context and Research.
- Be able to use ICT for their professional development.
- Leverage OERs for their teaching and research.
- Appreciate the role of ICT in teaching, learning and Research.
- Develop communication skills with special reference to Listening, Speaking, Reading and Writing.
- Learn how to use instructional technology effectively in a classroom.
- Master the preparation and implementation of teaching techniques.
- Develop adequate skills and competencies to organize seminar / conference / workshop / symposium / panel discussion.
- Develop skills in e-learning and technology integration.
- Have the ability to utilize Academic resources in India for their teaching.
- Have the mastery over communication process through the web.
- Develop different teaching skills for putting the content across to targeted audience.
- Have the ability to use technology for assessment in a classroom

PROGRAMME OUTCOMES:

- The scholars will develop knowledge and understand the current issues, research and developments.
- M.Phil Scholar shall get new ideas about the current scenario by studying literature.
- The scholars will acquire knowledge in soft skill and it can be introduced for class room teaching.

Research supervisor Papers

Course – IV CHEMICAL KINETICS

Research supervisor: Dr. A. Sekar

Unit – I

Empirical treatment of reaction rates: effect of concentration – rate expression – product study – stoichiometry. Experimental methods of measuring reaction rates: Instrumental method of analysis – chemical methods – determination of order. Relation between rate and mechanism.

Unit – II

Activated complex theory – current status – extension – applications. Entropy of activations – enthalpy of activation. Reactions in solutions: Factors determining reaction rates in solution. Reaction between ions, dipoles – effect of ionic strength – primary and secondary salt effect-kinetic isotope effect – primary and secondary isotope effect.

Unit – III

Complex reactions: steady state treatment – microscopic reversibility – detection and estimation of radicals in reaction system. Homogeneous catalyst in solution: Mechanism of acid – base catalysis – catalytic constant – general and specific and base catalysis. Bronsted catalysis law - acidity function.

Unit – IV

Hammett and Taft equation: Influence of substituent on reaction rates – electronic theory of organic reactivity – influence of substituent on the energy activation – LFER substituent constant reaction constant for aromatic and aliphatic systems. Applications of Hammett and Taft equations in reaction mechanism. Linear free energy relations and Bronsted catalysis law. Isokinetic relationship: Effect of temperature on reaction rates – reaction series – enthalpy and entropy relationship. Exner plot – isokinetic temperature.

Unit – V

Some reaction mechanism in solution: Hydrolysis of esters and acetals, oxidation of alcohols and aldehydes by N-halogeno compounds like NBS, NCS, CBT etc.

Text books

1. Laidler K.J, 1984, Chemical kinetics, 3rd edition, New Delhi, Tata McGraw-Hill Publishing Company.
2. Frost. A and Pearson R.G, 1970, Kinetics and Mechanism, John-Wiley Eastern.

References

1. Indian J. Chem., 1986. 25,pp 478.
2. Can. J. Chem., 1969. 47, pp 694.
3. Indian J. Chem. 1976. 14B, pp898.

Course –IV - Phytochemistry and Natural Products

Research supervisor :Dr. D. VijiSaralElezabeth

Unit I:Plants and Plant Products:

Classification of Plants – Nomenclature – Cells – Tissues – Structures and Functions of Cells and tissues – Primary Metabolites – Secondary Metabolites – Microorganism- Types – Microbes and Man – Biological Activities – Microbial Studies – Techniques – Interpretation of results

Unit II: Methods of Plant Analysis I:

Methods of Extraction – Cold Percolation Method – Soxhlet Method – Methods of Isolation – Methods of Separation Chromatography – Column Chromatography – Thin layer Chromatography – Gas Chromatography – High performance Liquid Chromatography– Distillations – Steam Distillation – Fractional Distillation – Vacuum Distillation – Crystallization Techniques

Unit III: Methods of Plant Analysis II:

UV-VIS spectroscopy – IR Spectroscopy – Proton and Carbon-13 NMR Spectroscopy – Mass Spectroscopy- GCMS Analysis– X-ray and Neutron Diffraction studies– Qualitative and Quantitative Analyses – Interpretation of Results

Unit IV: Phenolic Compounds and Terpenoids:

Methods of separation, isolation and identification – Phenolics – Phenyl propanoids – Anthocyanins – Flavonoids – Xanthenes – Stilbenes – Chemical conversions of these compounds – Structure Elucidation of Quercetin, Methods of separation, isolation and identification – Monoterpenes – Sesquiterpenes –Steroids – Carotenoids – Chemical conversions of these compounds – Structure Elucidation of Menthol. Alkaloids – Cyanogenic glycosides – Purines – Pyrimidines -Chemical conversions of these compounds

Unit V: Brief introduction to Pharmacological screening methods with following categories:

Hepatoprotective's, anti diabetes, antiepileptic, hypo lipidaemics, antioxidants, anti-inflammatory, analgesics & anticancer.

Text Books:

1. Peach K and Tracey MV (eds.), 1956-1964, *Modernederpfranzanalyse*, Berlin, Spingerverlag.
2. Krishnasamy N.R, 1999, *Chemistry or Natural Products*, Hyderabad, University Press.
3. Boyer RF, 1993, *Modern Experimental Biochemistry*, II Ed., California, The Benjamin /Cummings publishing company Inc.
4. Furniss BS, Hannaford AJ, Smith PWG and Tatchell AR, 1989, *Vogel's Text book of Practical Organic Chemistry*, V Ed., Essex, England, ELBS with Longman.
5. Harborne JB, 1988, *Phytochemical Methods: A Guide to Modern Techniques of Plant Analysis*, II Ed., London and New York, Chapman and Hall.

References:

1. Finar I.L. *Organic Chemistry*, Vol. 2. ELBS London.
2. Raphael Ikan, 1969, *Natural Products: A Laboratory Guide*, Jerusalem, Israel University Press.
3. Jeffrey C, 1982, *an Introduction Plant Taxonomy*, II Ed., Cambridge, Cambridge University Press.
4. William J and Sham M, 1976, *Microorganisms*, London, Mills and Boon Limited.
5. Ari Koskinen, 1993, *Asymmetric Synthesis of Natural Products*, Chichester, New York, Brisbane, Toronto, Singapore, John Wiley and Sons.

Course – IV- ADVANCED INORGANIC CHEMISTRY

Research supervisor: **Dr.M. Umadevi**

UNIT I – HEAVY METAL TOXICOLOGY

Concept, heavy metals in environment (i.e. Arsenic, Selenium, Cadmium, Mercury, Thallium, Lead), sources, toxicity, transformations, biochemical effects, and remedial measures

Organic pollutant toxicology: introduction, application potential, limitation of pesticides uses, toxicology of major pesticides, environmental impacts of pesticides, pesticide persistence, bioaccumulation and biomagnifications pesticide resistance

Radiation hazards: introduction, atomic radiations, natural radiations, effects of radiations, radioactivity and effects on man, impacts of radioactive radiations, radioactive waste, ionizing radiation and effects, radiation protection

UNIT – II COORDINATION COMPLEXES IN BIOLOGY AND MEDICINE

Metal-nucleic acid interactions:

The basics- nucleic acid structures- fundamental interactions with nucleic acids- fundamental reactions- binding of metal complexes with DNA- Techniques to monitor binding- applications of different metal complexes that bind nucleic acids (Spectroscopic probes).

Metal complexes in medicine:

Metal deficiency and diseases- toxic effects of metals- metals used for diagnosis and chemotherapy- platinum anticancer drugs- A case study of bioinorganic chemistry of platinum anticancer drugs- Design of new Inorganic anticancer drugs.

UNIT III -ELECTRON SPIN RESONANCE OF TRANSITION METAL IONS

EPR of transition metal ions containing one un paired electron- EPR of transition metal ions containing more than one un-paired electrons- Inter and Intra Kramer's transition- Solution, Powder and single crystal EPR Spectra – Study of distortion in geometry with the aid of EPR- EPR of Vanadyl, Mn(II), Fe(III), Cu(II) and Co(III) Complexes – Application of EPR in Biology and study of surface reactions over diamagnetic metal oxides.

UNIT IV - COMPUTATIONAL CHEMISTRY

Computational quantum chemistry - introduction – Ab initio calculations – Gaussian type orbital – Slater type orbital – basis set – Electron correlation – Hartree-Fock-Roothan SCF method for polyatomic molecules - Pariser-Parr-Pople approximation-configuration interaction-semi-empirical – Extended Huckel theory – Mulliken population analysis – Semi empirical SCF theory – computer programs - DFT the Kohn-Sham method – energy expression- orbitals – The DFT calculation procedure.

UNIT V - GREEN CHEMISTRY & NANOCHEMISTRY

Basic principles of green chemistry, Application of non-conventional techniques in organic synthesis (ultrasonic, microwave and grinding). Solid state synthesis and synthesis under solvent free conditions. Use of ionic liquids. **Drug discovery and development** A rational approach to drug design and drug development of following drugs: cimetidine oxamniquine. Nanoparticles and nanostructural materials – introduction – methods of preparation – application of nanoparticles: water purification – catalysis – sensors – information storage – solar cells – environmental cleanup – photodegradation of pesticides and photodisinfection of E.coli.

REFERENCES

Unit I

1. Perry, G. 1980. Introduction of Environmental Toxicology, Elsevier, Netherland.
2. Santra, S.C. 1994, Ecology; Basic and Applied, M.D. Publication, New Delhi (India).
3. Santra, S.C. 2001, Environmental Science, New Central Book Agency (P) Ltd. Calcutta (India).
4. Bertini, H.B. Gray, S.J. Lippard and J.S. Valentine, Bioinorganic Chemistry, University of Science, Mill Valley, California (1994)
5. J.D. Lee, Concise Inorganic Chemistry, 5th Edition, Blackwell Science (2000)
6. E.A.V. Ebsworth, D.W.H. Rankin and S. Craddock, Structural Methods in Inorganic Chemistry, ELBS, Great Brittan (1987)
7. D.F. Shriver, P.W. Atkins and C.H. Langford, Inorganic Chemistry, 3rd Edition, Oxford University Press (1999).

Unit II

1. R.S. Drago, Physical Methods in Chemistry, W.B. Saunders Co., London (1977).
2. B.J. Hathaway, D.E. Billing, *Coordin. Chem. Rev.*, **5**, 143 (1970).

3. G.H. Reed and G.D. Markham, in “*Biological Magnetic Resonance*” Vol. **6**, Berliner/Reuben, Plenum Press, New York, (1984) p. 73.
4. R .W. Hagen, *J. Chem. Soc. Dalton Trans.*, (2006) 4415
5. Instrumental Surface Analysis of Geological Material, VCH Publication , New York (1990)

Units III, IV & V.

1. M.T. Pope, and A. Muller, *Angew. Chem. Int. Ed. Engl.*, **30** (1991) 34.
2. L.C.W. Baker and D.C. Glick, *Chem. Rev.*,**98** (1998) 3.
3. M.T. Pope, in *Comprehensive Coordination Chemistry.*, G. Wilkinson, R.D. Gillard and J.A. McCleverty, (Eds,) Pergamon Press, New York, 3 (1987).
4. I.V. Kozhevnikov, *Chem. Rev.*, **98** (1998) 171.
5. R.A. Marcus and N. Sutin, *Inorg. Chem.*,**67** (1963) 853.
6. Y. Tajima, *Mini-Reviews in Medicinal Chem.*,**5** (2005) 255.
7. Computational Chemistry - Introduction to the theory and applications of Molecular and quantum mechanics, Errol Lewars, Springer Publisher, New Delhi.
8. Green Chemistry by M. Kidwai and V. K. Ahluwalia.
9. Wilson and Gisvold’s Text Book of organic medicinal and pharmaceutical chemistry Ed. R. F. Dorge.

Course - IV: COORDINATION CHEMISTRY AND SPECTROSCOPY

Research supervisor: Dr M. RAMESH

Unit I

Methods of preparation of coordination compounds - Analysis and determination of molecular formula - Volumetric, gravimetric and colorimetric methods - Conductance and magnetic measurements of complexes

Unit II

Theories of coordination - CF, MO, LF Theories - Merits and demerits - σ donor and π acceptor ligands - Carbonyls - Nitrosyls - Cyanides - Triphenyl phosphine complexes - Organo metallic compounds - Allene, alkyne and allyl complexes

Unit III

Special application to the study of coordination compounds - Electronic spectra - IR spectra - NMR spectra - ESR spectra - Moss Bauer spectra - PES

Unit IV

Kinetics and reaction mechanism in coordination compounds - SN_1 , SN_2 , SN_{CB} mechanisms - Trans effect - Electron transfer and electron exchange reactions - Catalysis by organometallic compounds

Unit V

Bioinorganic chemistry-structure and functions of chlorophyll, hemoglobin, myoglobin, cytochromes and iron enzymes

Text Books

1. Kettle SFA, Physical Inorganic Chemistry: A Coordination chemistry Approach, 1996, Oxford, Spectrum.
2. Drago R.S., 1977, Physical methods in inorganic chemistry, London, Saunders Golden Sunburst Series, W.B.Saunders Company.
3. Lewis J and Wilkinson RG (Editors), 1960, Modern coordination chemistry, Principles and Methods, New York, Interscience Publishers, Inc.

References

1. Lee JD, 1988, *Concise inorganic chemistry*, (sixth edition) London, ELBS.
2. Huheey JE., 1972, *Inorganic chemistry Principle structure and reactivity*, (second edition), New York, Harper & Row publishers.
3. Cotton F.A. and Wilkinson G., 1988, *Advanced inorganic chemistry*, (Third Edition) London, John Wiley & sons.

Course –IV Advanced Organic and medicinal Chemistry

Research supervisor: Dr. A. Idhayadhulla

Unit 1: Asymmetric synthesis:

Chiral auxiliaries, methods of asymmetric induction – substrate, reagent and catalyst controlled reactions; Analytical methods used for the determination of enantiomeric and diastereomeric excess; enantio-discrimination- HPLC, NMR, Optical rotation. Resolution - optical and kinetic resolution. Racemic modification and resolution of racemic mixture.

Unit 2: Ternary Mixture Separation:

Separation of at least ten mixtures containing three components. The mixtures should also involve separation of nitro phenols, amino acids, low boiling substances, water soluble substances. Amines, Phenols and acids used should also contain other elements and functional groups. The mixture separation should be carried out on micro-scale using ether. The purity of the separated compounds should be checked by TLC.

Unit 3: Two Dimensional NMR Correlation Spectroscopy:

Two dimensional NMR spectroscopy, 2D-HETCOR, ^1H - ^1H COSY, types of COSY experiments, 2D TOCSY, NOSEY, ROSEY, J resolved 2D NMR spectroscopy, HSQC, HMQC and HMBC.

Unit 4: Synthetic Methods in Organic Chemistry:

Transition metal complexes in organic synthesis: only Pd, Ni, Co, Pt, Fe, Rh, Ru; Grubb's catalyst, Ziegler Natta catalyst. Nitrogen, Phosphorous and Sulphur Ylides in Organic synthesis. **Designing in Organic Synthesis:** Retrosynthesis, disconnection, synthons, linear and convergent synthesis. **Coupling Reactions and Process:** Stills Coupling, Sonogashira reaction, Buchwald reaction, Pauson-Kahn Reaction, Suzuki Coupling, Mitsunobu reaction, Baylis-Hillman reaction, Mukiyama's esterification, Metathesis reaction. Green Chemistry – Basic Principles, Methods & Reactions.

Unit 5: Synthesis and application of Drugs from each of following class:

Antibiotics: Synthesis of Streptomycin, penicillins, cephalosporin-C, chloroamphenicol, tetracycline. **Antidiabetics:** Synthesis of Sequence of A- and B- chains of insulin, glibenclamide, metformin, ciglitazone. **Antivirals:** Synthesis of Acyclovir, amantidine, rimantidine and Zidovudine. **Cardiovascular drugs:** Synthesis of amyl nitrite, sorbitrate,

diltiazem, quinidine, verapamil, methyldopa, atenolol and oxrprenol. **Local Anti-infective agents:** Synthesis of sulphonamides, furazolidone, nalidixic acid, ciprofloxacin, dapsone, aminosalicylic acid, isoniazide, ethionamide, ethambutal, fluconazole, econazole, griseofulvin. **Antihypertension Drugs:** Antimalarial Drugs, Anti HIV Drugs, Anticancer Drugs

Text Books:

1. Organic Chemistry, by I. L. Finar, Vol8. 5th
2. Spectrometric identification of organic compounds, T. C. Morrill, R. S. Silverstein, G. C. Bessler 4th edition.
3. Comprehensive Organometallic Chemistry—G. Wilkinson, F.G.A. Stone and E. Abel Pergamon—1980.
4. Principles of Medicinal Chemistry (4th Edition) W. D. Foye, T. L. Lemke, D. A. Williams.

References

1. Principles and applications of asymmetric synthesis-Gou-Qiang Lin, YueMing Li and S. C. Chan-Wiley-Interscience, John Wiley and Sons, Inc. Publication 2001.
2. Vogel's, Practical Organic Chemistry.
3. Practical Organic Chemistry, R. K. Bansal
4. Some Modern methods of organic Synthesis, W. Carruthers.
5. Synthetic drugs—G. R. Chatwal—Himalaya, New Delhi 1995
6. Medicinal Chemistry—By A. Kar, Wiley, 2000.

Course –IV Organic and Bio-organic heterocyclic Chemistry

Research supervisor: R. Surendra Kumar

Unit – I Bioorganic Chemistry

Chemistry in bio systems – non covalent interaction and molecular recognition - proximity – enzymes chemistry – mechanism of enzyme action – chymotrypsin – transition state analogues – antibodies as enzymes – enzymes – enzymes in synthetic organic chemistry – coenzymes chemistry - biologic energy – ATP, NADH, NADPH and FADH₂ as electron carriers – coenzymes A as acyl carrier – suicide enzyme inactivators and affinity labels. Bioenergetics and metabolism – carbohydrate metabolism – lipid metabolism – citric acid cycle – urea cycle – link between glycolysis and citric acid cycle – biological oxidation.

Unit – II – Drug Design

Introduction, Analogues and Prodrug – Concept of Lead (Examples), Factors governing Drug Design, Relational approach to Drug-Design (Quantum mechanical approach, Molecular orbital approach, Molecular connectivity approach, Linear free energy approach). Drug Design: The method of variation (Drug design through disjunction, Drug Design through conjunction), Drug design and development: An overview (problem, Revolution in drug discovery, Research and development strategies, Molecular hybridization, Rigidity and flexibility vs Drug design (Increased rigidity and increased flexibility), Tailoring of drugs.

Unit – III Nature of bonding in Organic Molecules

Localized and delocalized covalent bond – Concept of aromaticity annulenes and hetero annulenes. Inductive and mesomeric effects, Huckel's rule for aromaticity in benzenoid and non-benzenoid compounds and anti-aromaticity and homo aromaticity. Introduction to types of organic reactions reactive intermediates.

Unit – IV - New synthetic Methodologies of Organic synthesis and applications of reagents.

Microwave and Ultrasonic methods of synthesis, biocatalysts and bio-transformations, phase-transfer catalyst, electro organic synthesis, Ionic liquids, Enantio and diastereoselective synthesis use of oxone. Designing of Organic synthesis (Retro synthesis) – Synthesis of heterocycles, agrochemicals, natural products and perfumery compounds – Synthesis and applications of the following drug: Cardiovascular, antidiabetics, antineoplastic and antiviral drugs – Computer aided drugs designing and molecular Modeling,.

Unit- V – Spectroscopy and Purification techniques

Basic principles of UV, IR, NMR and Mass spectroscopy – Instrumentation and applications of spectrometric methods in elucidating the structure of organic compounds. Chromatography: Principles and applications of Paper, Thin layer, 2D-thin layer chromatography, Gas chromatography – detectors, temperature programming, GC-MS, HPLC electro analytical methods – Principles and applications of electrogravimetry – Coulometry.

References:

Unit I :

A.L. Lehninger, Principles of Biochemistry, 5th edition, Freeman, W.H. & Company, New York, 2008.

Unit-II:

1. Medicinal chemistry; Ashutosh Kar, New age International Publisher.
2. Natural Products, Chemistry and Biological Significance, J. Mann, R.S. Davidson, J. B. Hobbs, D.V. Banthrope and J.B. Harborne, Longman, Essex.
3. New Trends in Natural Product Chemistry, Atta-ur-Rahman and M.I. Chaudhary Harwood Academic Publishers.
4. Organic Chemistry, Vol 2, I.L. Finar, ELBS

Unit:III

Organic Chemistry (fifth Edn.) by Morrison and Boyd, PHI, India

Unit-IV:

- 1] Modern Synthetic Reaction H.O. House:.
- 2] Principles of Organic Synthesis M.B. Smith:
- 3] (Organic Chemistry McGraw Hill) Hendrikson, Cram and Hammond:
- 4] Designing of Organic Synthesis S. Warren:
- 5] Organic Synthesis: Strategy and Control Warren and Wyatt:
- 6] The Total Synthesis of Natural Products Apsimon:
- 7] Organic Chemistry Vol. II and I. Finar 5th edition ELBS.

Unit-V:

1. Silverstein R.M., and W.P. Weber. Spectrometric identification of organic compounds. 2005.
2. Christian G.D. Analytical chemistry. 5th ed, John – Wiley and Sons Inc., 1994.

Course –IV ENVIRONMENTAL POLLUTION AND ADSORPTION

Research supervisor:: Dr. A. Kasthuri

Unit-1 Types of pollution

Types and causes of pollution – air pollution, water pollution, soil pollution, noise pollution, radioactive pollution, light pollution, thermal pollution. Effects of pollution. Environmental pollution in India.

Unit-2 Treatment methods

Physical processes: Sedimentation, flotation, filtration, centrifugal separation, screening.

Chemical processes: Precipitation, coagulation, oxidation and reduction, disinfection.

Sorption process: Adsorption, ion-exchange

Biological processes: Aerobic – fixed film and suspended growth processes, anaerobic process.

Membrane process: Electro dialysis, ultra-filtration, microfiltration, nano filtration, reverse osmosis.

Unit-3 Surface phenomena

Types of adsorption. Differentiation between physisorption and chemisorption. Factors affecting adsorption from solution. Applications of adsorbents and adsorption. Adsorption isotherm – Freundlich, Langmuir, B.E.T, Gibbs, Tempkin. Adsorption isobar.

Unit-4 Thermodynamics

Thermodynamic scale of temperature. Types of systems. Adiabatic and isothermal processes. Thermodynamic requirements of reactions - ΔG , ΔH , ΔS and their significance. Gibbs function and Helmholtz function as thermodynamic quantities. Equilibrium constant and free energy change. Thermodynamic interpretation of Le Chatelier principle. Addition on inert gases, reaction isotherms, Van't Hoff equation.

Unit-5 Kinetics

Introduction to rate equation, reaction order, molecularity and their characteristics. Derivation of rate constants for first order, second order and third order reactions; Dependence of temperature on reaction rate. Theories of reaction rate – Lindemann's theory of unimolecular reactions, collision theory of bimolecular gaseous reactions and absolute reaction rate theory

Text books:

1. S.S. Dara, A textbook of environmental chemistry and pollution control – S Chand & company, 2004.
2. Asim K. Das, Environmental chemistry with green chemistry, 2nd edition – New age int. publisher.
3. Tom Stephenson & Richard Stuetz, Principles of water and wastewater treatment process – 1st edition, IWA publishing, London, 2009.
4. Nicholas P Cheremisinoff, Handbook of water and wastewater treatment technologies – Butterworth-Heinemann, Woburn, 2002.
5. Gurdeep Raj, Advanced physical chemistry – Goel publishing house, 35th edition, 2009.
6. Keith J. Laidler, Chemical kinetics, 3rd edition, Pearson Education, 1987.
7. J. Rajaram J.C. Kuriacose, Thermodynamics – Dorling Kindersley (India) pvt. Ltd. 2013.

References:

1. P.S. Sindhu, Environmental chemistry –New age int. pvt. Ltd., 2010.
2. V.K. Ahluwalia, Green chemistry- Environmentally Benign Reaction – Ane books pvt. Ltd.,
3. Alfred Clark, Theories of adsorption and catalysis – Academic press, 1970.
4. B.R. Puri, L.R. Sharma & S. Pathania, Principles of physical chemistry – Vishal publishing company, 2008.