



UNIVERSITY OF CALICUT

Abstract

General and Academic - M Phil Programme in Chemistry at the Department of Chemistry in the University - Syllabus with effect from 2019 admissions - Implemented - Orders Issued

G & A - IV - J

U.O.No. 12652/2019/Admn

Dated, Calicut University.P.O, 19.09.2019

- Read:-*1. Item No. 4 in the minutes of the meeting of Board of Studies in Chemistry PG held on 26.06.2018
2. Item No. I.15 in the minutes of the meeting of Faculty of Science held on 30.06.2018
3. U.O.No. 5004/2019/Admn dated 04.04.2019
4. Item No. II.H in the minutes of the LXXVIII meeting of Academic Council held on 18.07.2018

ORDER

The meeting of Board of Studies in Chemistry PG resolved resolved vide paper read first above to approve the syllabus of MPhil Programme in Chemistry at the Department of Chemistry framed by the Department Council, with effect from 2019 admissions.

The decision of Board of Studies has been approved by the meeting of Faculty of Science vide paper read second above and then by the Academic Council vide paper read fourth above. The Rules and Regulations for M.Phil Programmes has been implemented in the University vide paper read third above.

Sanction has, therefore, been accorded to implement the syllabus of MPhil Programme in Chemistry in tune with the MPhil Regulations at the Department of Chemistry, in the University with effect from 2019 admissions.

Orders are issued accordingly. (Syllabus appended)

Biju George K

Assistant Registrar

To

HoD, Dept. of Chemistry

Copy to: Director, DoR/PS to VC/PA to PVC/PA to R/PA to CE/JCE V/DoA/SF/DF/FC

Forwarded / By Order

Section Officer

DEPARTMENT OF CHEMISTRY
UNIVERSITY OF CALICUT

M. PHIL. PROGRAMME IN CHEMISTRY
SYLLABUS

DEPARTMENT OF CHEMISTRY
UNIVERSITY OF CALICUT

M.Phil. Course in Chemistry

PROGRAMME OBJECTIVES:

The M.Phil. course in Chemistry aims to make the students capable of pursuing an independent research career by introducing the students with various research skills and equipping them with advanced knowledge in different areas of Chemistry.

Course Structure

Se m. No	Course Code	Name of the Course	Number of credits
I	CHE-M 001	Research Methodology	4
	CHE-M002	Analytical Methods	4
	CHE-M003	Advanced Inorganic Chemistry OR	4
	CHE-M004	Advanced Organic Chemistry OR	
CHE-M005	Advanced Physical Chemistry		
II	CHE-M006	Dissertation	20
Total Credits			32

SEMESTER : I

COURSE CODE : CHE-M001

COURSE TITLE : RESEARCH METHODOLOGY

CREDITS : 4

AIM: To familiarize the students with various steps involved in Chemistry and related area of research.

OBJECTIVES

- *To familiarize the students with an idea on how to select a research problem, and its design.*
- *To provide an idea on how to implement the research project, data collection, analysis and final reporting.*
- *To familiarize research ethics.*

COURSE CONTENT

MODULE I: Research objectives and types - Meaning of research-Motivation and objectives-Research methods Vs Methodology. Types of Research; Descriptive Vs Analytical. Applied Vs Fundamental. Quantitative Vs Qualitative, Conceptual Vs Empirical. Research formulation: Designing and formulating the research problem- Selecting the problem- Necessity of defining the problem- Formulation of a working Hypothesis- Importance of literature review in defining a problem- Literature Review- Primary and Secondary Sources- Reviews, treatise, monographs- patents- Web as a source- Searching the web and information mining- Critical literature review- Identifying gap areas from literature review.

MODULE II: Research design and methods - Basic principles involved- Need of research design- Features of good design- Important concepts relating to research design- Observation and facts, Laws and theories. Prediction and explanation, Induction, deduction. Development of models. Developing a research plan- Exploration, Description, Diagnosis, Experimentation. Determining experimental and sample design.

MODULE III: Data collection and analysis - Execution of the research- Observation and collection of experimental data. Methods of data collection-Sampling Methods- Sampling techniques, steps in sampling, sampling size, advantages and limitations of sampling- Data processing and Analysis strategies- Data analysis with Statistical Packages- Hypothesis-testing. Generalization and Interpretation. Applications and uses of common chemistry related software- Introduction to structure drawing, molecular modeling, computational chemistry, Cheminformatics and QSAR

MODULE IV: Research reporting and thesis writing - Structure and components of scientific reports- types of reports- technical reports and thesis significance- Different steps in the preparation- Layout, structure and language of typical reports- Data presentation- Illustrations, graphs, tables, histograms and pi diagrams- Bibliography, referencing and footnotes. Oral and poster presentation- Planning- Preparation- Practice- Making presentations- Use of visual aids.

MODULE V: Research ethics - Environmental impacts- Ethical issues- Ethical Committees- Commercialization- Copy right- royalty- intellectual property rights and patent law- Trade related aspects of Intellectual property rights- Reproduction of published materials- Plagiarism- Citation and acknowledgement- reproducibility and accountability- ethical committees

REFERENCES

- Frochim, W. M. K., *Research Methods: The Concise knowledge base*, Atomic Dog Publ.2005
- Garg, B. L.; Karadia, R.; Agarwal, F. and Agarwal, U. K., *An introduction to research methodology*, RBSA Publ, 2002.
- Kothari, C. R., *Research Methodolgy: Methods and Techniques*, New Age Intl, 1990.
- Sinha, S. C. and Dhiman, A. K., *Research Methodolgy, Vol I& II* Ess Ess Publ.2002.
- Wadehra, B. L., *Law relating to Patents, trademarks, copyright designs and geographical indications*, universal Law Publ, 2000.
- Carlos, C.M. , *Intellectual property rights, the WTO and developing countries. The Trips agreement and policy options*, Zed Books, New York, 2000.
- Coley, S. M. and Scheinberg, C. A. *Propasal writing*, Newbury stage, 1990.
- Day, R. A., *How to write and publish a scientific paper*, Cambridge Univ. 1992.
- Fink, A. *Conducting Research Literature reviews: From the internet to the Paper*. Sage 2009

- Graziano, A.M. and Rau, M. L. *Research methods: A process of inquiry*, Prentice, 2000.

SEMESTER : I

COURSE CODE : CHE-M002

COURSE TITLE : ANALYTICAL METHODS

CREDITS : 4

AIM: To familiarize the students with various sampling and analytical techniques involved in Chemistry related research.

OBJECTIVES

- *To familiarize the students with various methods for analyzing the data.*
- *To familiarize the students with chromatographic, spectroscopic and surface analysis techniques.*

COURSE CONTENT

MODULE I: Accuracy, precision and errors in chemical analysis-The mean and median- Standard deviation, variance and coefficient of variation-Determination of accuracy and precision of methods-Improvement of accuracy of analysis-Classification of errors-standard, systematic and random errors-Sources of error in analytical measurement -Errors in measuring signals-Propagation and minimization of errors -Repeatability, reproducibility, replication and documentation of experimental data. Approximation. Scatter diagram. Correlation coefficient-Analysis of variance ANOVA, Student "t" test. "f" test and "chi" square test, least squares analysis, weighted least squares analysis, confidence limits, correlation tables, linear regression coefficient, standard error of estimate, nonlinear regression, regression and ratio of variation.

MODULE II: Sampling techniques - Sample Preparation-Gas, Liquid and solid sampling-Sampling of air, water, soil, metallurgical, ore and mineral samples-Matrix

Effect-Pre-treatment of samples. Pre-concentration, evaporation, chelation, ion-exchange and solvent extraction-Speciation-Effect of speciation in chemical analysis. Pre-concentration and separation methods for speciation and detection. Speciation in water analysis.

MODULE III: Analytical techniques - Gas chromatography: Column efficiency and column equation -Capillary columns and packed columns HPLC-Basics and instrumentation ,Elution methods- Detectors in GC and HPLC-Absorption ,fluorescence, refractive index, electrochemical, radioactivity, evaporative light scattering detectors .Supercritical fluid chromatography-Ion chromatography-Chiral Column Chromatography-Capillary Electrophoresis -Hyphenated Systems-MS as a detector in chromatography-GC-MS,LC-MS-Evolved gas analysis by GC. Analysis of CO_x, SO_x, and NO_x in air, Analysis of pesticide residues in environmental and biological samples. Analysis of metals by AAS, AFS and NAA.

MODULE IV: Spectroscopic techniques - Structure Elucidation of compounds based on UV, IR, ¹H and ¹³C NMR, ESR and Mass spectral techniques. Introduction to 2D and other NMR methods-NOE, APT, DEPT, HOMO and HETEROCOSY, FAB, MALDI, ESI, APPI, SIMS and Tandem (MS/MS) techniques- Use of electronic. IR, NMR, Mossbauer and ESR in the structure elucidation of inorganic and coordination compounds.

MODULE V: Surface analysis techniques - Analysis of Surfaces-Surface preparation-principle, Instrumentation and applications of SIMS, AES, XPS and ESCA- Microscopy and probe techniques. Instrumentation and applications of SEM, TEM, STM, AFM, Scanning, Nearfield Optical Microscopy SNOM, Scanning Ion Conducting Microscopy (SICM), Ellipsometry. Neutron Scattering and XRD methods.

REFERENCES

- Day, R. A. and Underwood, A. L., *Quantitative Analysis*, Printice Hall 1985.
- Pavia, D. L., Lampman, G. M. and Kriz, G. S., *Introduction to Spectroscopy*, Saunders

- Skoog, D. A. and West, M., *Fundamentals of Analytical Chemistry*, Saunders 1996
- Vogel, A. I., *Textbook of Quantitative Inorganic Analysis*, E L B S 1962
- Williams, D. H. and Fleming, I. , *Spectroscopic Methods in Organic Chemistry*, Mc Graw Hill
- Willard, H. H., Merritt, L. L., Dean, J. A. and Settle, F. A., *Instrumental Methods of Analysis*, 6th Edn, CBS

SEMESTER : I

COURSE CODE : CHE-003

COURSE TITLE : ADVANCED TOPICS IN INORGANIC CHEMISTRY

CREDITS : 4

AIM: To familiarize the students with various advanced topics of Inorganic Chemistry

OBJECTIVES

- *To give an in-depth knowledge in bioinorganic chemistry.*
- *To familiarize the students with inorganic synthesis, organometallic reactions, and inorganic photochemistry.*

COURSE CONTENT

MODULE I: Metal ions in biology-sites of coordination in biomolecules and biopolymers - electronic geometrical structures - ion transport and storage in cellular systems - ionophores activated transport-ion pumps-Sodium and Calcium pump. Alkali metals and regulation of membrane potentials -Role of Ca²⁺ in blood clotting and Mg²⁺ in phosphate transfer - Bioenergetics -ATP cycle-Metal complexes in biomedicine - chelators, drugs, contrast agents, radiotracers.

MODULE II: - Redox enzymes, metalloenzymes and metalloproteins- Ca, Cu, Mg, Fe, Mo and Fe-S enzymes and proteins - storage and transport of Fe, V and other

metal ions - ferritin, transferrin, hemosiderin, ceruloplasmin and siderophores. Transport of oxygen by Heme and Non-heme oxygen carriers -hemerythrin, hemocyanin, hemovanadin - Nature of heme - dioxygen binding in hemoglobin and myoglobin- cooperativity in hemoglobin -cytochromes, peroxidases and catalases - carboxypeptidase A, carbonic anhydrase, metallothionein-Nitrogenases, N₂ fixation and its model systems -

MODULE III: Reactivity of coordinated ligands- Small molecules addition and activation -Reaction involving O₂, CO, CO₂, SO₂, NO₂, H₂, alkenes and alkynes addition and activation-oxidative addition, reductive elimination and insertion reactions. Catalysis, general principles. Homogeneous catalysis, catalytic, Hydroformylation and oxidation of alkenes, asymmetric hydrogenation, Monsanto acetic acid manufacture process. Catalytic application of palladium. Heterogenous catalysis- the nature of catalyst, catalytic ammonia synthesis, SO₂ oxidation-Zeolite based heterogenous catalysis

MODULE IV: Special techniques for inorganic synthesis- vacuum line, plasmas, photochemical and electrolytic methods, synthesis of BCl₃, AlF₃, SiF₄, NF₃, OF₂, S₂Cl₂, BrF₃, SbF₃, SF₄, and N₂F₄. Synthesis of transition metal complexes involving the following methods- Electron transfer reaction, substitution reaction, reactions of coordinated ligands, aldol condensation, imine bromination, hydrolysis, substitution exchange reaction, template effect and macrocyclic ligands.

MODULE V: MO Theory of coordination compounds. Tetrahedral octahedral and square planar complexes with and without pi- bonding. Reaction mechanism of coordination compounds. Eigen-Wilkins equation and Fuoess-Eigen equation. Marcus theory of coordination compounds. Inorganic photochemistry - Photo substitution, redox, dissociation and isomerization reactions. Adamson 'rule. Photochemistry of Chromium, cobalt and Rhodium complexes. Photosensitization. Photoreactions and solar energy conversions-Chlorophyll and photosynthesis. Photosystem I and II system mimicking water splitting and CO₂ reduction

REFERENCES

- Adamson, A.W. and Fleischaner, P. D. Concepts of Inorganic Photochemistry, Wiley.
- Blazani, V. and Carassiri, V. Photochemistry of Coordination Compounds, Academic.
- Cotton, F. A.; Wilkinson, G.; Murillo, C. A. and Bochmann, M. Advanced Inorganic Chemistry, Wiley, 1999.
- Cowan, J. A. Inorganic Biochemistry- An Introduction, VCH.
- Fenton, D. E. Biocoordination Chemistry, Oxford Univ. Press, 1995.
- Lippard, S. L.; Berry G. M. Principles of Bioinorganic Chemistry, University Science, 1997.
- Tobe, M. L. and Burgess J. Inorganic Reaction Mechanisms, Longmans, 1999.
- Wilkins, R. G. Kinetics and Mechanism of Reactions of Transition Metal Complexes, 2nd Edn, VCH.
- Bertini, I.; Gray, H. B.; Lippard, S. J. and Valentine, J. S. Bioinorganic Chemistry, University Science, 1994.
- Crabtree, R. H. The organometallic Chemistry of Transition Metals, 2nd Edn, Wiley.
- Hay, R. W., Bioinorganic Chemistry, Ellis Harwood, 1984.
- Parkins, A. W. and Poller, R. C. An Introduction to Organometallic Chemistry, Macmillan.

SEMESTER : I

COURSE CODE : CHE-004

COURSE TITLE : ADVANCED TOPICS IN ORGANIC CHEMISTRY

CREDITS : 4

AIM: To familiarize the students with various advanced topics of Organic Chemistry

OBJECTIVES

- *To give an in-depth knowledge in organic synthetic techniques.*

- *To familiarize the students with molecular recognition, supramolecular chemistry and green chemistry.*

COURSE CONTENT

MODULE I: Techniques in organic synthesis - Synthetic planning, disconnections, synthons and retrosynthetic analysis. Functional group interconversions FGI - Protection and deprotection strategies for amino, hydroxy, carbonyl and carboxyl groups- Baldwin's rules for cyclisation - Synthesis of small and large carbocyclic rings- C-C and C=C bond forming reactions - Heck, Stille, Suzuki, Kumada, Sonogashira, Peterson and McMurray reactions-Metathesis reactions - Ring closing metathesis (RCM), Ring opening metathesis (ROMP), Cross metathesis (CM) Acyclic diene metathesis (ADMP) - Introduction to multicomponent reactions: Ugi, Passerini, Biginelli and Strecker reactions.

MODULE II: Molecular recognition - Noncovalent interactions and their significance in molecular recognition and supramolecular chemistry - codon and anticodon recognition, protein biosynthesis - Introduction to MR based chemo and biosensors - Introduction to DNA sequencing and PCR - Introduction to molecular devices and Nano chemistry.

MODULE III: Supramolecular chemistry - Design of molecular receptors based on host-guest interaction - Molecular receptors. Calixarenes, cryptands, crown ethers, carcerands, cyclophanes, cyclodextrins and other molecular hosts. Self assembly of supramolecular structures.

MODULE IV: The concept and development of green chemistry - Significance of waste minimization - redesign of organic reactions - The metrics of greenness: AE - Examples of green laboratory and industrial processes - Organic synthesis using alternative energy inputs: microwave and sonochemical synthesis. Synthesis using solvent less or alternate media conditions: supercritical fluid, fluorous and ionic liquid media - Introduction to solid phase organic synthesis - Support materials and

matrices - Polymeric and other supported reagents. Principles of combinatorial synthesis.

MODULE V: Green catalysts - Solid Acids: Clays, Zeolites and Mesoporous materials, Montmorillonite-K10 and KCF, Zeolite - MCM 41, ZSM 5, Zeolite Y, Nafion H and superacids - Applications of solid Acids and Envirocatalysis in Friedel-Crafts acylations and alkylations, esterifications, oxidations, aromatic electrophilic substitutions. Enzymes and immobilized enzymes in organic synthesis - Supported catalysts.

REFERENCES

- Ahluwalia, V. K. and Aggarwal, R., *Organic Synthesis: Special Techniques*, Narosa
- Anastas, P. T. and Warner, J. C., *Green Chemistry: Theory and Practice*, Oxford Univ. Press.
- Bansal, R. K., *Synthetic Applications in Organic Chemistry*, Narosa
- Jenkins, P. R., *Organometallic Reagents in Synthesis*, Oxford Univ. Press
- Lehn, J.-M., *Supramolecular Chemistry*, VCH.
- Mackie, R. K.; Smith, D. M. and Aitken, R. A., *Guidebook to Organic Synthesis*, 3 Edn. Longman
- Sanghvi, R. and Srivastava, M. M., *Green Chemistry*, Narosa
- Turrett, N. K., *Combinatorial Synthesis*, Oxford Univ. Press

ADDITIONAL READINGS

- Cattrall, R. W., *Chemical Sciences*, Oxford Univ. Press.
- Clark, J. H., *Catalysis of Organic Reactions by Supported Inorganic Reagents*, VCH 1994
- Clark, J. H., *The Chemistry of Waste Minimization*, Blackie Academic 1995
- Clark, J. H. and Macquarrie, D., *Handbook of Green Chemistry and Technology*, Blackwell 2002

- Dugas, H., *Bioinorganic Chemistry*, 3rd Edn, Springer.
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- Norman, R. O. C., and Coxon, A., *Modern Synthetic Reactions*, Chapman And Hall.
- Smith, M. B., *Organic Synthesis*, 2nd Edn. Mc Graw Hill.
- Vogtle, F., *Supramolecular Chemistry*, Wiley.
- Zhuj And Bienayme, H. (Ed) *Multicomponent Reactions*, Wiley V C H 2005

SEMESTER : I

COURSE CODE : CHE-005

COURSE TITLE : ADVANCED TOPICS IN PHYSICAL CHEMISTRY

CREDITS : 4

AIM: To familiarize the students with various advanced topics of Physical Chemistry

OBJECTIVES

- *To give an in-depth knowledge in quantum mechanics*
- *To familiarize the students with advanced topics of surface science, nanomaterials and electrochemistry.*

COURSE CONTENT

MODULE I: Schrodinger wave equation in Cartesian coordinate - Separation of variables and solution of the equation for energy and wave function - Particle in a three-dimensional box - Hydrogen atom- Total wave function - H orbitals and their shape - Perturbation theory, first order correction to energy application to an harmonic oscillator - Time dependent perturbation theory - SCF and variation method - Secular determinant.

MODULE II: Perturbation and variation methods for He - Second order perturbation theory - Stark effect - Time dependent perturbation theory - Antisymmetric of wave functions - Slater determinants - Hartree - Fock equations - Hund's rules - Atomic spectra - R-S coupling - Born - Oppenheimer approximation - Exchange integral - Single and triplet states - electronic states of diatomic molecules - Wave functions for nuclear and electronic motion - Separation of vibrational, rotational and translations parts - Selection rule for the rigid rotor and the harmonic oscillator - Selection rules in electronic spectroscopy.

MODULE III: External and internal surfaces of solids - Microporosity and microporous materials - Structure of surface- techniques for the study of surfaces - Gas-solid and solid-liquid interfaces - Methods, techniques and instrumentation in surface science - Adsorption and general purpose of adsorption isotherms - Classes of determination - Introduction to nano science and technology - Effects of dimensionality on the properties of solids - Behavior of electrons in crystalline solids - Semiconductor nanostructures: classification, transport mechanism and excitonic effects.

MODULE IV: Nano materials: Dimensionality - Size effects and size dependent properties - CNTs, quantum dots, nano clusters and nano particles - core shell nanoparticles - principles of self assembly - stabilization of nano particles - methods of synthesis - top- down methods - photo, optical and particle beam lithographics - probe lithography - Bottom-up methods - self assembly of monolayers, directed and layer by layer assembly- Pattern replication methods - soft and nanoimprint lithography. Pattern transfer methods - sol gel process, colloids, hydrolytic methods, precipitation and condensation reactions - Gelation- gel network- xero gels - aero gels - Electrochemical; Physical and chemical vapor depositions - MEB and LB films - Chemical modification of nano surfaces - nano sized porous materials - nano - ceramics

MODULE V: The electrochemical Double layer, Gibbs absorption isotherm, electrocapillarity equations – Models for double layer: Helmboltz, Gouy- Chapman and Stern. Electrode potentials and thermodynamics – Kinetics of Electrode reactions and models based on electrochemical potentials, the exchange current, current- overpotential equation and its approximate forms – Mass transfer equation, migration during electrolysis, effects of supporting electrolyte. Diffusion random walk model, Ficks laws – Electroanalytical techniques – Voltammetry at a microelectrode – d.c. polarography, Ilkovic equation – pulse and differential pulse polarography. Chronopotentiometry, Chroamperometry and Chronocoulometry, coulostatic methods. Hydrodynamic methods, the convective diffusion equation, rotating disk electrode, current potential curves. Impedance techniques. Ac Voltammetry.

REFERENCES

- Adamson, A. W., The Physical chemistry of surface, 4th Edn, Wiley, 1994.
- Atkins, P. W., Molecular Quantum Mechanics, 2nd Edn, Oxford Univ. Press. 1983.
- Fletcher, D., Industrial Electrochemistry, Blackie Academic, 1982.
- McQuarrie, D. A., Quantum Chemistry, Oxford Univ. Press, 1983.
- Ozin, G. A. and Arsenault, A. C., Nanochemistry, RSC Publ, 2008.
- Pilar, F. L., Elementary Quantum Chemistry, McGraw Hill, 1980.
- Poole, C. P. and Owens, F. J., Introduction to Nanotechnology, Wiley, 2007.
- Somorjai, G. A., Introduction to Surface Chemistry AND Catalysis, Wiley, 2007.

SEMESTER : II

COURSE CODE : CHE-006

COURSE TITLE : Dissertation

CREDITS : 20

AIM: To make the students competent to perform a specific research project in Chemistry.

OBJECTIVES

- *To implement the research methods studied in the theory course.*
- *To familiarize the students with various techniques to solve a chemical problem in hand.*
- *To enhance the soft skills of students in communication and problem solving.*
- *To perform a scientific research work in a time bound fashion.*

QUESTION PATTERN FOR M.PHIL. COURSE

- A. One very short answer type question from each unit of the paper(5x2=10)
- B. One Short answer type question from each unit of the paper (4x5=20)
- C. One essay type question from each unit. This question can have subdivisions (a) and (b) with 5 marks each also. Four full questions are to be answered. (10x4=40)

