UNIVERSITY OF KERALA

MASTER OF PHILOSOPHY

PROGRAMME IN CHEMISTRY

SYLLABUS AND SCHEME

FOR THE PROGRAMME AND EVALUATION

FOR 2016 ADMISSIONS ONWARDS

UNIVERSITY OF KERALA

2016

MASTER OF PHILOSOPHY PROGRAMME IN CHEMISTRY

FOR 2016 ADMISSIONS ONWARDS

PROGRAMME STRUCTURE

The master of philosophy programme in Chemistry covers one academic year consisting of two semesters of six months each. The syllabus will come to effect for admissions in the 2016 academic year onwards in the University Department. The programme consists of a total of four courses, of which three are Lecture-based courses. The project work includes a dissertation that is to be submitted at the end of the second semester and on the date announced by the University.

Scheme of Examinations

There shall be two core courses which are common to all the candidates and an elective course to be selected from three choices. The examinations for Courses I, II and III shall be conducted at the end of Semester I and the viva-voce for Course IV (Dissertation) shall be conducted at the end of Semester II as per the Regulations for the M. Phil. programme of the University.

Evaluation and Grading

Sem	Title of Courses	Contact Hrs/Sem	Examination	
			Duration Hrs	Credits Max.
I	Course I –CHE711-Research Methodology	92	3	4
	Course II –CHE712 – Analytical Methods	92	3	4
	Course III –CHE713 (i) -Selected Topics in Inorganic Chemistry OR CHE713 (ii) -Selected Topics in Organic Chemistry OR CHE713 (iii) -Selected Topics in Physical Chemistry	92	3	4
II	Course IV – CHE721 – Dissertation and Viva-voce based on project and dissertation	Dissertation + Viva-Voce		20

COURSE I

CHE 711 RESEARCH METHODOLOGY

UNIT 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

UNIT II 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.

UNIT III RESEARCH DESIGN, METHODS

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

UNIT IV RESEARCH- 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, Chem informatics and QSAR

UNIT V 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.

UNIT VI 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

1. Garg. B L, Karadia R, Agarwal F and Agarwal U K, *An introduction to research methodology*, RBSA Publ, 2002.

2. Kothari C R, *Research Methodolgy: Methods and Techniques*, New Age Intl, 1990.
3. Sinha S C and Dhiman A K, *Research Methodolgy, Vol I& II* Ess Ess Publ.2002.
4. Frochim W M K, *Research Methods: The Concise knowledge base*, Atomic Dog Publ.2005
5. Wadehra B L, *Law relating to Patents, trademarks, copyright designs and geographical indications,* universal Law Publ, 2000.

Additional Readings

1. Graziano A M and M L Rau, M L. *Research methods: A processof inquiry*, Prenice, 2000.
2. Carlos c M, *Intellectual property rights, the WTO and developing countries. The Trips agreement and policy options*, Zed Books, New York, 2000.
3. Coley S M and Scheinberg C A. *Propasal writing*, Newbury stage, 1990.
4. Day RA , *How to write and publish a scientific paper*, Cambridge Univ. 1992
5. Fink A. *Conducting Research Literature reviews*: *From the internet to the Paper*. Sage 2009

COURSE II –

CHE712-ANALYTICAL METHODS

UNIT I-TREATMENT OF ANALYTICAL DATA –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.

UNIT II- TREATMENT OF ANALYTICAL DATA –II

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.

UNIT III- 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. Preconcentration and separation methods for speciation and detection. Speciation in water analysis.

UNIT-IV-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 NOx in air, Analysis of pesticide residues in environmental and biological samples. Analysis of metals by AAS,AFS and NAA.

UNIT V- SPECTROSCOPIC TECHNIQUES

Structure Elucidation of compounds based on UV,IR, ^{1}H and ^{13}C 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.

UNIT VI- 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, Near field Optical Microscopy SNOM, Scanning Ion Conducting Microscopy (SICM), Ellipsometry. Neutron Scattering and XRD methods.

REFERENCES

1. Day R A and Underwood A L, *Quantitative Analysis*, Printice Hall 1985
2. Willard H H, Merritt L L, Dean J A and Settle F A, *Instrumental Methods of Analysis*, 6th Edn, CBS
3. Pavia D L, Lampman G M and Kriz G S, *Introduction to Spectroscopy*, Saunders
4. Williams D H and Fleming I , *Spectroscopic Methods in Organic Chemistry*, Mc Graw Hill
5. Vogel A I, *Textbook of Quantitative Inorganic Analysis*, E L B S 1962
6. Skoog D A and West M, *Fundamentals of Analytical Chemistry*, Saunders 1996

COURSE III –

CHE 713 (i) SELECTED TOPICS IN INORGANIC CHEMISTRY

UNIT I BIOINORGANIC CHEMISTRY I

Metal ions in biology-sites of coordination in biomolecules and biopolymers - electronic geometrical structures - ion transport and srorage in cellular systems - ionophores activatedtransport-ion pumps-sodium pump - redox enzymes, metalloenzymes and metalloprotiens- 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

UNIT II BIOINORGANIC CHEMISTRY II

Transport of oxygen by Heme and Nonheme 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, N_2 fixation and its model systems – alkali metals and regulation of membrane potentials –Role of Ca^{2+} in blood clotting and Mg^{2+}

in phosphate transfer – Bioenergetics -ATP cycle-Metal complexes in biomedicine – chelators, drugs, contrast agents, radiotracers.

UNIT III ORGANOMETALLIC REACTIONS

Reactivity of coordinated ligands- Small molecules addition and activation –Reaction involving O_2,CO,CO_2,SO_2,NO_2, H_2, 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, SO_2 oxidation-Zeolite based heterogenous catalysis

UNIT IV INORGANIC SYNTHESIS

Special techniques for inorganic synthesis- vacuum line, plasmas, photochemical and electrolytic methods, synthesis of BCl_3,AlF_3, SiF_4, NF_3,OF_2, S_2Cl_3 , BrF_3,SbF_3,SF_4,and N_2F_4. 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.

UNIT V INORGANIC SYNTHESIS AND PHOTOCHEMISTRY

Inorganic photochemistry – Photo substitution, redox, dissociation and isomerization reactions. Photoreactions and solar energy conversions-Chlorophyll and photosynthesis. Photosystem I and II system mimicking water splitting and CO_2 reduction

REFERENCES

1. Cotton F. A., Wilkinson G., Murillo C. A. and Bochmann M. Advanced Inorganic Chemistry, Wiley, 1999.
2. Cowan J. A. Inorganic Biochemistry- An Introduction, VCH.
3. Wilkins R. G. Kinetics and Mechanism of Reactions of Transition Metal Complexes, 2nd Edn, VCH.
4. Tobe, M. L., and Burgess J. Inorganic Reaction Mechanisms, Longmans, 1999.
5. Lippard, S. L., Berry G. M. Principles of Bioinorganic Chemistry, University Science, 1997.
6. Fenton D. E. Biocoordination Chemistry, Oxford Univ. Press, 1995.
7. Blazani, V. and Carassiri, V. Photochemistry of Coordination Compounds, Academic.
8. Adamson A.W. and Fleischaner P. D. Concepts of Inorganic Photochemistry, Wiley.

ADDITIONAL READING

1. Bertini I. Gray H. B., Lippard S. J. and Valentine J. S. Bioinorganic Chemistry, University Science, 1994.
2. Hay R. W., Bioinorganic Chemistry, Ellis Harwood, 1984.
3. Crabtree R. H. The organometallic Chemistry of Transition Metals, 2nd Edn, Wiley.
4. Parkins A. W. and Poller R. C. An Introduction to Organometallic Chemistry, Macmillan.

COURSE III

CHE 713 (ii)-SELECTED TOPICS IN ORGANIC CHEMISTRY

UNIT 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 carbocyling rings-Newer C-C and C=C bond forming reactions-Heck.Stille,Suzuki,Kumuda,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.Passerni,Petasis Biginelli and Strecker reactions.

UNIT II MOLECULAR RECOGNITION

Noncovalent interactions and their signifinificance in molecular recognition and supramolecular chemistry-Molecular recognition in codon and anticodon recognition and in cellular protein biosynthesis-Introduction to MR based chemo and biosensors-Introduction to dideoxy DNA sequencing and PCR-Introduction to molecular devices and nanochemistry.

UNIT III-SUPRAMOLECULAR CHEMISTRY

Design of molecular receptors based on host-guest interaction-Molecular receptors.Calixaranes,cryptands,crowns,carcerands,cyclophanes,cyclodextrins and other molecular hosts.Self assembly of supramolecular structures.

UNIT IV-GREEN CHEMISTRY I

The concept and development of green chemistry-Significance of waste minimisation-redesign of organic reactions-The metrics of greenness:AE etc-Examples of green laboratory and industrial processes-Organic synthesis using alternative energy inputs:microwave and sonochemical synthesis.Synthesis using solventless or alternate media conditions :superclritical 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.

UNIT V-GREEN CHEMISTRY II

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 Envirocatsin Friedal-Crafts acylations and alkylations,esterifications,oxidations,aromatic electrophilic substitutions.Enzymes and immobilized enzymes in organic synthesis-Supported catalysts.

REFERENCES

1. Mackie R K. Smith D M and Aitken R A, *Guidebook to Organic Synthesis*, 3 Edn. Longman
2. Ahluwalia V K and Aggarwal R, *Organic Synthesis: Special Techniques*, Narosa
3. Lehn, J-M, *Supramolecular Chemistry*, VCH.
4. Anastas P T and Warner J C, *Green Chemistry: Theory and Practice*, Oxford Univ. pres.

5. Sanghvi, R and Srivastava M M, *Green Chemistry*, Narosa
6. Turrett N K, *Combinatorial Synthesis*, Oxford Univ. Press
7. Bansal R K, *Synthetic Applications in Organic Chemistry*, Narosa
8. Jenkins P r, *Organomatallic Reagents in Synthesis*, Oxford Univ. Press

ADDITIONAL READINGS

1. Vogtle F, *Supramolecular Chemistry*, Wiley.
2. Dugas H, *Bioinorganic Chemistry*, 3rd Edn, Springer.
3. Norman R O C, and Coxon A, *Modern Synthetic Reactions*, Chapman And Hall
4. Cattrall R W, *Chemical Sciences*,Oxford Univ. Press
5. Smith M B, *Organic Synthesis*, 2nd Edn. Mc Graw Hill
6. Clark J H, *Catalysis of Organic Reactions by Supported Inorganic Reagents*, VCH 1994
7. Zhuj And Bienayme H (Ed) *Multicomponent Reactions*, Wiley V C H 2005
8. Kurti L and Czako B, *Strategic Applications of Name Reactions in Organic Sythesis*, Elseiver 2005
9. Clark J H and Macquarrie D, *Handbook of Green Chemistry and Technology*, Blackwell 2002
10. Clark J H, *The Chemistry of Waste Minimization*, Blackie Academic 1995

COURSE III
CHE 713 (iii) SELECTED TOPICS IN PHYSICAL CHEMISTRY

UNIT I - QUATUM MECHANICS – 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 anharmonic oscillator – Time dependent perturbation theory – SCF and variation method – Secular determinant.

UNIT II - QUATUM MECHANICS – II

Perturbation and variation methods for He – Second order perturbation theory – Stark effect – Time dependent perturbation theory – Antisymmetry 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.

UNIT III - SURFACE SCIENCE

External and internal surfaces of solids – Microporosity and microporous materials – Structure of surface p-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 – Behaviour of electrons in crystalline solids – Semiconductor nanostructures: classification, transport mechanism and excitonic effects.

UNIT IV - NANO MATERIALS

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 lithographies - 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 vapour depositions – MEB and LB films – Chemical modification of nano surfaces – nano sized porous materials – nano – ceramics

UNIT V - ELECTROCHEMISTRY

The electrochemical Double layer, Gibbs absorption isotherm, electrocapillarity equations – Models for double layer: Helmboltz, Gouy- Champman 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. Impedence techniques. Ac Voltammetry.

REFERENCES

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