

HAJEE KARUTHA ROWTHER HOWDIA COLLEGE

(An Autonomous Institution Affiliated to Madurai Kamaraj University, Madurai)

Re- Accredited with "A" Grade by NAAC

Uthamapalayam – 625533



DEPARTMENT OF CHEMISTRY

Master of Philosophy – Chemistry

Syllabus

(Academic Year 2017 -18 Onwards)

Program Specific Outcome

PSO1: Strategise opportunity to get jobs in quality control labs, Pharmaceutical companies and in various industries

PSO2: Envisage research ideas to do research at an advanced level in the Divergent fields of chemistry

PSO3: Sought viable options to start pharmaceutical and chemical industries

I Semester

Theory Papers	Code
Paper I– Research Methodology	– 17MCHC11
Paper II– Course Work	– 17MCHC12
Paper III– Optional Paper (Elective)	
Advances in Chemistry	– 17MCHE11
Or	
Advanced Inorganic chemistry	– 17MCHE12

Scheme of Examinations under Choice Based Credit System

Term End Examinations (TEE)	– 60 Marks
Continuous Internal Assessment Examinations (CIAE)	– 40 Marks
Total	– 100 Marks

Pattern of Continuous Internal Assessment Examinations (CIAE)

Average of Two Internal Tests (each 25 marks)	– 25 Marks
Seminar	– 15 Marks
Total	– 40 Marks

Pattern of Term End Examinations

(Max. Marks: 60 / Time: 3 Hours)

Part A (5 x 6 = 30 marks)

Answer **ALL** questions choosing either (a) or (b)

(One question from each unit with internal choice)

Part B (3 x 10 = 30 marks)

Answer **ANY THREE** questions out of five questions

(One question from each unit)

II Semester**Dissertation only- 200 marks**

Evaluation of dissertation – 150 marks
(Average of internal and external examiners)

Viva- voce – 50 marks

DETAILS OF COURSE CATEGORY, CODE, TITLE & CREDITS

Course Category	Course Code	Course Title	Hrs/ Week	CIAE Marks	TEE Marks	Max. Marks	Credits
SEMESTER - I							
Core - I	17MCHC11	Research Methodology	5	40	60	100	4
Core - II	17MCHC12	Course Work	5	40	60	100	4
Elective	17MCHE11	Advances in Chemistry	5	40	60	100	4
	17MCHE12	Advanced Inorganic chemistry					
			15			300	12
SEMESTER - II							
Core	17MCHCEV	Project	Internal		External		
		Dissertation	$\frac{150 + 150}{2}$			150	8
		Viva- voce	-		50	50	
						200	8
Grand Total						500	20

RESEARCH METHODOLOGY

Programme : **M. Phil. Chemistry**

Part : Core – I

Semester : I

Hours : 5

Subject Code : **17MCHC11**

Credits : 4

Course Outcomes

CO1: To Know the primary and secondary sources in literature survey

CO2: To Understand the concept of documentations in thesis writing

CO3: To Learn the needs of various tests in error analysis

CO4: To Study the C language and its applications in chemistry

CO5: To Ascertain various instrumentation methods

UNIT – I - Literature search

Searching the chemical literature, primary sources- journals and patents, secondary sources- Beilstein, reviews, periodicals-serials-monograph and text books, dictionaries, encyclopedias, catalogues and index of tabulated data, location data, location of published and comprehensive account of research with special reference to physical, organic and inorganic chemistry. Inductive and deductive reasoning- role of experimentation- interpretation of results- formation- testing and rejection of hypothesis- Getting idea on impact factor of journals- Leading funding agencies in India- Submission of research project proposals.

UNIT – II – Thesis writing

Thesis layout: Format of title page, certificates, declaration, Preface, acknowledgements and table contents. Text of the thesis: Chapter division and subdivision-use of centered heading, side heading and paragraph heading. Quotations: When, what and how to use quotations, interpolation of quotations. Footnotes, tables and figures: Format, conventions and referencing. Documentation: Methodology of writing references-MLA and APA style. Editing and evaluating: Basic idea of editing, revising and evaluating the thesis. Ethics and research Plagiarism.

UNIT – III – Error in Chemical Analysis and Statistics

Classification of errors-accuracy-precision-minimization of errors-mean-standard deviation- Normal or Gaussian distribution-Reliability of results-Confidence interval-comparison of results- Student's t-test,F test, paired t-test-correlation and regression-the least square method for deriving calibration plots like straight line-Analysis of variance (ANOVA)- Pearson correlation coefficient-r value.

UNIT – IV – Computers in chemistry

Data types: int, short, long int, float, double and long double;variable and scope.Global automatic register and static operators: assignment, caching, precedence and associativity:program selection:if-else logical operators-ternary operator switch statement:Repetition:while.do-while and for loops, goto statement;functions, void. Return statement, invoking functions,passing arguments-prototyping.

Array: Single dimensional arrays,accessing arrays,initializing and copying arrays-array as function arguments-multidimensional arrays.

Simple C programming applications in chemistry such as van der waals equation, pH titration, kinetics, radioactive decay, evaluation of lattice energy and ionic radii from experimental data. Use of computer in literature search, significance of chemdraw-drawing chemical structure-paste them in the text.

UNIT – V – Analytical Chemistry

Electro Chemical methods: Voltammetry – principles-linear sweep voltammetry-cyclic voltammetry, differential pulse voltammetry-electrodes and electrolytes- pulse polarographic methods-applications.

Principles and instrumentations of Atomic Force Microscopy(AFM), powder XRD,Scanning Electron Microscopy(SEM), Transmission Electron Microscopy (TEM)and HRTEM, Scanning Tunneling Spectroscopy(STS), Scanning Tunneling Microscopy(STM), Thermo gravimetric Analysis(TGA), Differential Thermal Analysis(DTA), Differential Scanning Colorimetry(DSC)

BOOKS RECOMMENDED

- ♦ Jerry March, Advanced organic chemistry, 4th edition.
- ♦ Robert E Maizll, How to find chemical information? A guide for practicing chemistry teachers and students.
- ♦ F.AbdulRahim, Thesis writing – A Manual for researchers, First edition, New Age International (P) Ltd., New Delhi, 1996.
- ♦ R. Laurie, Guide to Writing Great Research Papers, First Edition, McGraw Hill, New York, 1999.
- ♦ Vogel's textbook of Quantitative Chemical Analysis, 5thEdn., Longman scientific and Industrial, UK, 1989.
- ♦ D.A.Skoog, D.M.West&F.J.Holler, Fundamentals of Analytical Chemistry, VII Edn., Saunder's College of publishing, Newyork.
- ♦ K.V.Raman, Computers in chemistry, Tata McGraw-Hill publishing Co.,Ltd., New Delhi (1993).
- ♦ E.Balagurusamy, Programming in ANSI-C, II Edn., Tata McGraw-Hill publishing Co.,Ltd New Delhi (1998).
- ♦ J. Mendham, R.C. Denney, J.D. Barennes, and M.J.K. Thomas, Vogel's textbook of Quantitative Chemical Analysis, 6thEdn., Pearson education, New Delhi, 2004.
- ♦ D.A.Skoog, D.M.West, J.F. Holler and S.R. Crouch, Fundamentals of Analytical Chemistry, VIIIEdn, Thomas AsiaPvt Ltd., Singapore, 2006.
- ♦ H.H. Willard, L.L. Merrit, J.A. Dean, F.A. Jr. Settle, Instrumental Methods of Analysis, 7th Edition CBS Publishers and Distributors, New Delhi, 2008.
- ♦ Micro machines as Tool for Nano Technology, Chapters 5&8, Springer-Verlag Berlin Heilderberg, 2003.

COURSE WORK

Programme	: M. Phil. Chemistry	Part	: Core – II
Semester	: I	Hours	: 5
Subject Code	: 17MCHC12	Credits	: 4

Course Outcomes

CO1: To study group theory and its applications

CO2: To get an idea of toxicity and uses of metals

CO3: To ascertain retro synthetic analysis and organometallic reagents

CO4: To know the mechanism of various reactions

CO5: To develop the skills for interpretation of inorganic complexes using spectroscopy

Unit I– Group Theory

Projection operators – symmetry adapted linear combination (SALC) – construction of MO wave functions for allyl, butadiene, cyclopropenyl, benzene and tetramethylcyclobutane calculation of delocalization of hybrid orbitals and wave functions of hybrid orbitals for molecules having tetrahedral, trigonal triangular and square planar geometry (SP^2 , SP^3 and dSP^2 hybridizations).

Application of group theory to IR, Raman and UV spectroscopy - selection rules for fundamental vibrations – symmetry of normal vibrations of molecules belonging to C_{2h} , C_{2v} , C_{3v} , C_{4v} , D_{3h} , D_{4h} , $D_{\infty h}$ and $C_{\infty v}$ point groups, stretching mode analysis of metal carbonyls and metal complexes.

Unit II – Metal ions in medicine:

Introduction-Trace elements- diseases due to metal deficiencies and excess -Toxic effects of heavy metals(Pb,Cd, Hg and As) and their detoxification-Metals used for diagnosis and chemotherapy-inorganic compounds as therapeutic agents- anti arthritis drugs – anti -cancer drugs -Platinum anti-cancer drugs: discovery,principles and development of drugs- Clinical picture of cisplatin and carboplatin-Bioinorganic chemistry of platinum anticancer drugs-design of new inorganic anticancer drugs.

Unit III–Organic Synthesis and Organometallic reagents in synthesis:

Types of (carbon to carbon forming) reactions-Key intermediates-starting materials-Sandheimer synthesis-Stork approach. Use of retrosynthetic analysis for the synthesis of simple cyclic molecules- Gabriel synthesis. A schematic analysis of the total synthesis of γ -caprolactone, 6-methoxy tryptamine, 6,6-ethylenedioxy-1(9)octalin-2-one. α -onocerin and quinoto copper reagents – vinyl Grignard reagents – carboalumination-nucleophilic addition of alkenyl anions and alkyl nitriles to carbonyl compounds – ortholithiation – use of formamidines-lithiated dithianes and nitroalkanes in synthesis.

Unit IV – Molecular Rearrangements and selective name reactions

Bamberger rearrangement- Amadori rearrangement- Baker Venkataraman rearrangement- Brook rearrangement- Von Richter rearrangement- Carrol rearrangement- Fischer-Hepp rearrangement- Tiemann rearrangement-peterson's synthesis- Vilsmeier-Hack reaction-Dakin reaction- Allan-Robinson reaction-Hell- Volhard- Zelinsky reaction-Shapiro reaction- Pechmann reaction.

Unit V - Instrumental methods of analysis

Basic instrumentation, principle of EPR spectrometer and its applications. Combined applications of Mass, UV-VIS, IR leading to structural elucidation of Inorganic complexes. Monitoring the DNA binding by UV, IR, NMR and CV spectral techniques. Applications of different metal complexes that bind nucleic acid.

BOOKS RECOMMENDED

- ♦ F.A.Cotton, Chemical Applications of Group Theory.
- ♦ G.Davidson, Introduction to Group Theory.
- ♦ R. S. Drago, Physical Methods in Chemistry.
- ♦ V. Ramakrishnan and Gopinath, Group Theory in Chemistry.
- ♦ IavanoBertini, Harry B. Gray, Stephen J. Lippard and Joan Selverstone valentine, Bioinorganic chemistry, Viva Books Pvt. Ltd., 1998.
- ♦ James E. Hugheey, Ellen A. Keitler and Richard L. Keitler, Inorganic Chemistry, 4th Edn, Harper COLLinsCOLlege Publishes, New York, 1993.
- ♦ J. Chem. Edn., November 1985.
- ♦ F. A. Cotton and G. Wilkinson, "Advanced Inorganic Chemistry", 5th Edition, John Wiley&Sons, Singapore, 1998.
- ♦ A.K. Das, A text book on medicinal aspects of bioinorganic chemistry, CBS Publishers.
- ♦ K. De, Environmental chemistry, Wiley Eastern Ltd., Meerut, 1994.
- ♦ G.R. Chatwal and Ajay Kumar Bhagi, Bioinorganic chemistry, Himalaya Publishing House.
- ♦ R.E. Ireland, Organic Synthesis, Prentice-Hall of India Pvt. Ltd., 1969.
- ♦ W. L. Jolly, The Synthesis and characterization of Inorganic compounds.
- ♦ D. M. Adams & J. B. Raynor, Advanced practical Inorganic chemistry.
- ♦ G. Brahmachari, Organic Naming Reactions (A unified approach), First Edition, Narosa Publishing House, New Delhi, 2006.
- ♦ J. March, Advanced Organic Chemistry, (Appendix A) Sixth Edition, John Wiley & Sons, New Delhi, 2007.
- ♦ R. S. Drago, Physical Methods in In Organic Chemistry.
- ♦ John R. Dyer. Application of adsorption Spectroscopy, Prentice- Hall.
- ♦ William Kemp, Organics Spectroscopy. ELBS, 3rdEdn.
- ♦ Robert M. Silverstein, Francis X. Webster, Spectrometric Identification of Organic compounds, 6thEdn., John Wiley & Sons, Inc., 2004.

ADVANCES IN CHEMISTRY
(OPTIONAL PAPER – 1)

Programme : M. Phil. Chemistry	Part : Elective –I
Semester : I	Hours : 5
Subject Code : 17MCHE11	Credits : 4

Course Outcomes

- CO1:** To ascertain the various principles of adsorption
- CO2:** To learn the identification and structural elucidation of pigments
- CO3:** To study the different methods of corrosion prevention
- CO4:** To develop the skills for interpretation of organic compounds using NMR spectroscopy
- CO5:** To know the photo physical process of different transition metal complexes

Unit 1- Surface chemistry

The solid liquid interface. Adsorption from solution – adsorption of polymers. adsorption in binary liquid systems : adsorption at the solid – solution interface – heat of adsorption at the solid-solution interface. adsorption of electrolytes : stern – layer adsorption – counter ion adsorption – ion exchange . photophysics and photochemistry of the adsorbed state . photo chemistry at the solid – solution interface .

Unit II- Natural products

Selection of plants – extraction – preparation techniques of column, TLC, preparative TLC- Soxhlet extraction – crystallization methods –colour reactions, identification and structural elucidation (by UV, IR, H^1NMR , $C^{13}NMR$ and Mass spectra) of glycosides, anthocyanins – flavones – flavanols – isoflavones – flavanoids – quercetin, tannins - naphthoquinones – steroids – terpenoids- bio active studies – organisms – MLC - MIC – biosynthesis of non- nitrogenous metabolites from Shikimicacid, flavanoids and related polyphenols .

Unit III- Corrosion

Definition of corrosion-corrosion damage-cost of corrosion-historical background-classification of corrosion-Factors influencing corrosion-Theories of corrosion-Electrochemical theory-The basic electrochemical process- Mechanism of electrochemical reaction-Thermodynamics of corrosion-Potential –pH diagram –Methods of corrosion prevention and control- corrosion control by inhibitors and their inhibition action-Classification of corrosion inhibitors-Theories of corrosion inhibition-Adsorption theory-Hydrogen over potential theory-Film formation theory-Methods of studying inhibitors-Non electrochemical methods-Gas volumetric method-Weight loss method-Electrochemical methods-Polarization method-Determination of surface coverage-Spectroscopic methods-Biocidal methods-Other methods SEM,AFM.

Unit IV- NUCLEAR MAGNETIC RESONANCE

Nuclear spin states – nuclear magnetic moments – absorption of energy – mechanism of absorption (Resonance) – instrumentation and sample handling – comparison of NMR spectra at low and high field strength – chemical shift – spin-spin interaction – complex spin-spin interaction – chemical exchange – deuterium substitution – shielding mechanisms – coupling constant – vicinal and germinal coupling – long range coupling – magnetic anisotropy – double irradiation – simplification of complex proton NMR spectra – shift reagents – mechanics of measurements – ^1H NMR spectra of alkanes, alkenes, alkynes, aromatic compounds – ketones, esters and carboxylic acids.

^{13}C spectra – proton coupled ^{13}C spectra – spin-spin splitting of ^{13}C signals – proton decoupled ^{13}C spectra – DEPT – 45, 90 and 135 techniques – H–H COSY, C–H COSY, NOESY, HMBC, TOCSY and off-resonance decoupling.

Assigning structure to the following compounds using the above techniques – epoxides, pyrazolines, pyrans and pyrimidines.

Unit V- Photochemistry

Photophysics of transition metal complexes using di-imine ligands. Comparison of absorption spectra of different complexes of same metal using homoleptic and hetero-leptic ligands. Phenomenon of fluorescence – Jablonsky diagram-mirror image rule and Frank – Condon principle. Fluorescence lifetimes and quantum yields-Fluorescence quenching.Stern- Volmer equation and its derivation. Photo induced ET reactions of di-imine metal complexes of Iron, Ruthenium and Osmium using phenols and amines as quenchers. Study of microheterogeneous systems - Structure and characteristics of micelles (CTAB, SDS and Triton -X 100) and Reverse micelles like AOT in organic solvent.

BOOKS RECOMMENDED

- ♦ A.W. Adamson and A.P. Gast, Physical Chemistry of Surfaces, Sixth Edition, India Pvt. Ltd., New Delhi, 1997.
- ♦ J.S. Gamble-Flora of the Presidency of Madras, Volume I, II and III – (1967), II Reprinted Edition, Botanical survey of India, Calcutta.
- ♦ I.L. Finar – Organic Chemistry Volume II, Fifth Edition.
- ♦ B.P. Pandey – Tannins and Dyes, S. Chand Company, 1981.
- ♦ J. Bassett, R.C. Denney, G.H. Jeffery and J. Mendham, Vogels Text Book of Quantitative Inorganic Analysis, Fourth Edition, ELBS, 1985.
- ♦ R.M. Silverstein, G.C. Bassler and T.C. Morrill, Spectroscopic identification of organic compounds, Sixth Edition, McGraw Hill, New York (2006).
- ♦ K.L. Mukherjee, Medical Lab Technology, Second Volume, 1988.
- ♦ Anantha Narayanan and Panickar, Text Book of Microbiology, Fifth Edition, 2003.
- ♦ M.G. Fontana and N.D. Greens, "corrosion engineering", MC Graw Hill, New York (1978)
- ♦ G. Wranglen, "An introduction to corrosion and protection of metals" Chapman and Hall, New York (1985)
- ♦ H.H. Uhlig and R. Winston, "Corrosion and corrosion control" John Wiley and sons (1985).
- ♦ Silverstein, Bassler and Morrill. Spectroscopic identification of organic compounds, IV Edn.
- ♦ Doland L. Pavia, Gary M. Lampmann and George S. Kriz, Introduction to Spectroscopy.
- ♦ John R. Dyer, Applications of absorption spectroscopy of organic compounds.
- ♦ William Kemp, Organic spectroscopy.
- ♦ K. Kalyanasundaram, Photochemistry Polypyridine and Porphyrin Complexes. Academic Press: London, 1992.
- ♦ Principles of Fluorescence Spectroscopy, Second Edition by Joseph R. Lakowicz.
- ♦ Photochemistry by Rohathi and Muherji.

ADVANCED INORGANIC CHEMISTRY**(OPTIONAL PAPER – II)**

Programme	: M. Phil. Chemistry	Part	: Elective –II
Semester	: I	Hours	: 5
Subject Code	: 17MCHE12	Credits	: 4

Course Outcomes

- CO1:** To study about the various inorganic polymers and their properties
- CO2:** To know the reactions of coordinated ligands
- CO3:** To learn bonding, synthesis and reactions of organometallic compounds
- CO4:** To understand the interaction of metal ions with DNA and characterization
- CO5:** To ascertain various forms of energy and their utilisation

Unit I – Inorganic polymers

General properties of inorganic polymers – classification – homoatomic – heteroatomic – condensation – addition polymers – coordination polymers. Glass transition temperature – phosphorous based polymers – polydimethoxy and polydiethoxyphosphazines – polyphosphoryl chlorides – polyphosphates – metaphosphates – poly phosphates cross linked phosphates – ultra phosphate glasses – borophosphate glasses – uses of phosphorous polymers – polymeric sulphur nitride – chalcogenide glasses – coordination polymers – chain polymers – twodimensional polymers – synthetic coordination polymers – polymers having phthalocyanide and related structure – polymers with bis chelating agents.

Unit II – Molecular rearrangement and reactions of coordinated ligands:

Molecular rearrangement of four coordinated complexes – six coordinated complexes – reaction at coordinated ligands – reaction due to metal ion polarization of coordinated ligands – hydrolysis of amino acid esters and amides and of peptides – Aldol condensation – imine formation, hydrolysis and substituent exchange – the template effect and macrocyclic ligands.

Unit III - Organometallic compounds:

Alkylidene and alkylidyne complexes – synthesis of alkylidene complexes in low oxidation state and higher oxidation state of metals – synthesis of alkylidyne complexes – reactivity and bonding in alkylidene and alkylidyne complexes – alkyne complexes – synthesis reactivity and bonding – cobalt catalysed alkyne cycloaddition reactions.

Unit IV –Bio – inorganic chemistry:

Metalloproteins and enzymes – blue copper proteins - copper proteins as oxidases/reductases – nickel containing enzymes structure of DNA – types of nucleic acid interactions – coordination, intercalation and hydrogen bonding – interactions of metal ions with nucleic acid – redox chemistry, hydrolytic chemistry – monitoring the DNA binding by UV, IR, NMR and CV spectral techniques. Applications of different metal complexes that bind nucleic acid – conformational probes – metallo foot printing reagents. Nature's use of metal/ nucleic acid interactions. Metal ion toxicity – detoxication using chelating agents. Inorganic compounds as therapeutic agents. Anticancer drugs – antiarthritis drugs. Treatment of essential trace metal deficiencies and excess.

Unit V – Energy and environment

Sources of energy – fossil fuels – nuclear fission – nuclear fusion – solar energy in space heating and water heating – production of electricity using solar energy – solar trough collectors – power tower – solar bond – solar energy for driving vehicles – power from indirect solar energy – hydropower, wind power, biomass energy – product of ethanol, methane from biomass – photosynthesis – photoelectrochemical cells – geothermal energy – ocean thermal energy conversion – tidal power, air energy.

BOOKS RECOMMENDED

- ♦ B. R. Puri, L. R. Sharma and K. C. Kalia, Principles of inorganic chemistry, Milestone publishers, Delhi, 30th edition.
- ♦ Gurdeepraj, Advanced inorganic chemistry, Goel publishing House
- ♦ K.F.Purcel and J.C.kotz, Inorganic chemistry.
- ♦ R.C.Mehotra and A.Singh, Organometallic chemistry.
- ♦ Manfred Bochmann, Organometallics I Complexes with transition metal carbon s-bonds.
- ♦ IvanoBertini, Harry B.Gray, Stephen J. Lippard and Joan Selverstone Valentine, Bioinorganic chemistry, Viva Books Pvt.Ltd., 1998.
- ♦ A.K.De, Environmental chemistry, Wiley Eastern Ltd.,
- ♦ A.K.Das, A text book of Medicinal aspects of Bioinorganic chemistry, CBS publishers.
- ♦ S.S. Dara, A textbook of environmental chemistry and pollution control, S. Chand & Co 7th edition.

DISSERTATION

Programme : **M. Phil. Chemistry**

Semester : **II**

Course Code : **17MCHCEV**

Part: **Dissertation**

Hours: **6**

Credits: **8**

Course Outcomes

CO1: Formulate a research a topic

CO2: Familiar with the various stages of research process

CO3: Carried out projects in different fields of chemistry

In the II semester the students have to write a dissertation.

Regular attendance is compulsory.

(200 marks: Dissertation 150 and Viva voce 50)