PERIYAR UNIVERSITY PERIYAR PALKALAI NAGAR SALEM – 636 011



DEGREE OF MASTER OF PHILOSOPHY CHOICE BASED CREDIT SYSTEM SYLLABUS FOR BRANCH IV (M) M.PHIL. CHEMISTRY FOR THE STUDENTS ADMITTED FROM THE ACADEMIC YEAR 2012 – 2013 ONWARDS

Sl. No	Sem	Course (Paper)	Paper Code	Title of the Paper	Exam Hours	I	E	Т	C
Core Courses									
1.		Course-I		Scientific Research and Methodology	3	25	75	100	4
2.	Ι	Course-II		Elective Paper: Spectroscopic and Instrumental Methods in Chemical Investigations	3	25	75	100	4
3.		Course-III		Background Research Paper (Guide Paper)	3	25	75	100	4
4.	II	Dissertation / Project Work		Dissertation		*50	#150	200	12
Total						500	24		

* 50 Marks – Viva-Voce

150 Marks - Dissertations

Scheme of Examinations:

Paper I, II and III do end of the first semester

Paper III Conducted in the Department

Max.Marks: 100 Marks Minimum Passing: 50 Marks

Dissertation / Project work: Second Semester

Viva voce: Conducted by the Department by the External & Internal Examiners.

Question paper Pattern for University Examination

Time: 3 Hours Max.Marks - 75

PART-A: 5x5=25

(Answer all questions)

(One question from each unit with internal choice)

- 1. (a) or (b)
- 2. (a) or (b)
- 3. (a) or (b)
- 4. (a) or (b)
- 5. (a) or (b)

PAPER-B: 5x10=50

(Answer all questions)

(One question from each unit with internal choice)

- 6. (a) or (b)
- 7. (a) or (b)

- 8. (a) or (b) 9. (a) or (b) 10. (a) or (b)

CORE PAPERS

PAPER-I

SCIENTIFIC RESEARCH AND METHODOLOGY

UNIT-I Survey of Literature

Primary sources – Journals, Papers, reviews, communications, notes, patents, Journals of different fields of Chemistry (Organic, Inorganic, Physical, Polymer, Pharmaceutical, Industrial and Analytical)

Secondary Sources –Titles, importance of categorization and their importance, Abbreviations of names, Nomenclature of compounds and their usage.

Abstracts –Types (Chemical, Physical, Analytical), Survey of abstract indexes (substance index, author index, general technique index, collective and comprehensive indices), Beiestein compounds and tables of information. Chemical abstract search through loaded CDS. Aids of Computer devices in literature survey.

Selection of topic and facilities - Selection of specific topics of research laboratory and instrumental facilities -location of journals, e-mail address, specific articles of science citation cards and indices, summerisation of works already done and published in the chosen field.

UNIT-II Proposal, Paper and Thesis Writing

Assignments and test papers, Thesis and dissertations, style and conventions in writing, selection of topic.

Rough drafting of the article – Tile, Abstract, Introduction, Literature review problem and time limitation, Experimental methods, Results and discussions, Foot notes, Figures, Data presentations, Tables, Sign convention followed – Biblography, Conclusions and recommendations.

The general format – page and chapter format – use of quotations – foot note – tables and figures. Results and discussions – applicability of the findings to common usage – referencing – abbreviations used etc.

UNIT-III Statistical Analysis of Data

Various types of errors – precision and accuracy – significant figures, various statistical tests on the accuracy of results, positive and negative deviation from accurate results - the Gaussian distribution – the normal distribution of random errors, mean value, variance and standard deviation, reliability interval, deviations from the Gaussian law of error distribution, t-tests-comparison of the mean with the expected value, comparison of the results of two different methods, comparison of the precision of two methods by F-test, Gross errors and elimination of outlying results, graphical methods – Linear regression, regression line, standard deviation, correlation coefficient – Multiple Linear regression (one variable with two other variables)

UNIT-IV Introduction to Computing and Networking

Introduction to computers and computing – hardware, Basic organization of a computer, CPU, Main memory, Secondary storage, I/O device, Software, System and application software, High and low level languages, Compilers, Algorithms and Flow charts.

Introduction to networking – Computer networks, Network components, Hubs, switches, repeaters, routers, bridges and gateways – LAN, WAN, internet and internet worldwide web, internet for chemists – online search of chemistry databases, e-journals, search engines for chemistry, chemweb.

UNIT-V C – Programming

Structure of a C program – Data types, Constants and Variables, Keywords, Operators and Expression.

Control structure – if, if-else, nested if-else, while, while-do, for, nested for, goto, continue, break, switch case statements.

REFERENCE BOOKS

- J.Anderson, B.H.Durston and M.Poole, "Thesis and Assignment Writing", John Wiley, Sydney 1970.
- 2. R. Berry, "How to Write a Research Paper", Pergamon, 1969
- 3. Ralph Berry, "The Research Project: How to Write It", Fourth Edition Routledge (UK), 2000.

- 4. W.G. Campbell, "Form **and Style in thesis writing**", Boston M.A; Houghton Mifflin Co., 1970.
- 5. J.Anderson, "Thesis and Assignment Writing", Wilely, 1970.
- 6. Jerry March, "Advanced Organic Chemistry: Reactions, Mechanisms And Structure," 5th ed., Wiley, 1996
- 7. A.I. Vogel, "Quantitative Inorganic Analysis", 3rd Ed., ELBS Longman London.
- 8. D.A.Skoog and D.M.West, **Fundamentals of Analytical Chemistry**, Holt Rinehart and Winston Publications, IV Edn, 1982.
- 9. W.L. Cochran, "**Statistical Methods**", Oxford and IBH Publication, New Delhi, (1967).
- 10. K. Balagurusamy, "**Fortran for Beginners**", Tata McGraw Hill, New Delhi, 1990.
- 11. K.V. Raman, "Computer in Chemistry", Tata McGraw Hill, New Delhi, 1993.
- 12. K. Balagurusamy C++, Tata McGraw Hill, New Delhi, 1995.
- 13. Sanjay Saxena, MS OFFICE 2000
- 14. Manual of MS Office Microsoft inc.

PAPER –II

SPECTROSCOPIC AND INSTRUMENTAL METHODS IN CHEMICAL INVESTIGATIONS

Hours	L	T	P	С
72	4	0	0	4

UNIT-I Spectroscopy -I

Nuclear Magnetic Resonance Spectroscopy - Theory, Instrumentation of ¹H NMR and ¹³C NMR - Chemical shift, coupling,; Applications – Nuclear resonance in solids and liquids, resolution – Double resonance methods – spin relaxation modes, etc.

Electron Spin Resonance Spectroscopy – Principles, Instrumentation, Hyperfine splittings. Interpretation of spectra's, solid, liquid and solution state spectral studies; Anisotropicsystem – the triplet state; Theory of G-tensor, ESR of transition metal ions and complexes; Endor and Eldor techniques.

UNIT-II Spectroscopy -II

Mass spectra - Principles of Mass Spectroscopy - Presentation and analyses of Spectra - Fragmentation process - McLafforty rearrangement - Aprotoontics.

Mossbauer Spectroscopy – The Mossbauer effect, experimental methods, Hyperfine interaction, parameters for Mossbauer spectra, applications, molecular and electronic structures. Solid state chemistry – conversion electron Mossbauer spectroscopy.

UNIT-III Spectroscopy - III

FT – IR – Basic principles, Instrumentations and applications

Fluorescence Spectroscopy – Fluorophore lit tome and its measurement – Fluorescence anisotropy – Fluorescence correlation spectroscopy application in biological systems.

Vibrational Spectroscopy – Molecular vibrations - IR and Raman Techniques – Vibrational Spectra and Symmetry, Assignment of bands - Structural informations - Group frequencies - use of isotopes - resonance Raman spectroscopy.

UNIT-IV Spectroscopy - IV

Atomic absorption Spectroscopy –Theory, Forbidden transitions and Selections, space quantisation, Zeeman effect, the Paschen-Back effect, the Stark effect, spectral line width, the Back-Goudsmith effect, applications.

Electronic and Photoelectron Spectroscopy – Excitation and ejection of electrons, electronic energy levels, core n level PES, Symmetry of molecular orbitals, valence levels PES, Applications - transition metal complexes.

X-ray Spectroscopy – Principles, instrumentation, X-rays fluorescence, absorption and diffraction methods. The electron microscope – non-dispersive X-ray absorption.

X-rays diffraction methods – Polymerization characteristics, Particle size determination.

UNIT-V Electroanalytical Techniques

Polarography – Theory, DME and importance, Current Voltage curves, Diffusion current and its theory, factors affection it. Polarographic wave and half wave potentials, applications. Oscillographic Polarography, Square wave polarography, Tensimetry.

. Chronopotentiometry - Cyclic Voltammetry, Amperometry, theoretical principles, applications in chemical investigations.

Electrogravimetry – Principles and applications.

REFERENCE BOOKS:

- 1. William Kemp, **NMR in Chemistry**, Mac Millan, 1986.
- 2. A.Carrington, A.D. Melahlam, **Introduction to Magnetic Resonance**, Harper and Row, New York, 1967.
- 3. E.A.V.Ebsworth, David, W.H.Ranklin and Stephen Cradock, **Structural methods in inorganic chemistry,** Black well Scientific Publ., 1987.
- 4. R. Drago, **Physical methods in chemistry**, Reinhold, New York, 1968.

- 5. C.N.Banwell, **Fundamentals of molecular spectroscopy,** McGraw Hill, New York, 1966.
- 6. J.R.Dyer, **Applications of absorption spectroscopy of organic compounds**, Prentice Hall of India Pvt. Ltd., New Delhi, 1974.
- 7. G.W.Ewing, **Instrumental methods of chemical analysis**, McGraw Hill Pub, 1975.
- 8. Doughlas. A.Skoog, **Principles of instrumental analysis**, Saunders College Pub.Co, III Edn., 1985
- 9. R.C. Kappor and B.S. Agarwal, **Principles of polarography**, Wiley Eastern Ltd., 1991.
- 10. J.R.Lackowicz, Fluorescence Spectroscopy
- 11. Fundamental of Photochemistry by K.K.Rohatgi Mukherjet.

PAPER -III - (GUIDE PAPER)

BACKGROUND RESEARCH PAPER

This background paper should be related to the proposed research work towards the dissertation. The Guide will give the syllabus.

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PART II

DISSERTATION

Candidates shall carry out research work in consultation with the guide/supervisor and submit the dissertation to the University through the Supervisor and Head of the Department at the end of the year from the commencement of the course which shall be valued by internal examiner (supervisor) and one external examiner appointed by the University from a panel of four names sent by the Supervisor through the Head of the Department at the time of submitting the dissertation.

M.Phil DEGREE EXAMINATION CBCS PATTERN

CHEMISTRY – II SEMSTER

DISSERTATION / PROJECT WORK

DISSERTATION : 150 Marks

VIVA VOCE : 50 Marks TOTAL : 200 Marks

Model Question Paper

M.Phil., Degree – Branch IV (M) Chemistry

(For the candidates admitted from 2012-2013 onwards)

SCIENTIFIC RESEARCH AND METHODOLOGY

Time: Three Hours Maximum:75 marks

Answer All Questions

All questions carry equal marks

Part - A (5x5=25 marks)

1. (a) Describe how chemical abstract is useful in literature survey of your research work.

(or)

- (b) "If the subject index is proper, the weightages given to substance index and formula index can be reduced" Justify this statement with an example
- 2. (a) Write an account of selection of topic for a research work

(or)

- (b) Describe the principles of research work.
- 3. (a) Explain the Gaussian distribution with a suitable diagram.

(or)

(b) The amount of oxalic acid present in a given solution was determined by two different methods, one standard and the other new, when the following results were obtained:

Sample Number Amount of oxalic acid (g/lit) determined by

bumple rumber rimbult of oxume dela (g/m) deter					
	Standard Method	New Method			
1.	8.65	9.35			
2.	4.70	11.06			
3.	7.35	8.90			
4.	13.95	12.58			
5.	17.26	18.99			
6.	12.80	11.72			

show that is no significant difference between the two methods.

4. (a). Write a note on high and low level languages.

(or

- (b) Give a brief note on network compounds.
- 5. (a) Explain the structure of a c program.

(or

(b) Discuss the syntax of switch case statement.

Part-B (5x10=50 Marks)

6. (a) Describe the manuscript preparation, formats used to publish a research in Indian journal of Chemistry.	h paper
(or)	
(b) Discuss about the aids of computer devices in literature survey.	
7. (a) Give an account of the general format of a thesis.	
(or)	
 (b) i) How will you prepare a manuscript entitled "Photoreduced election t reactions of Ruthenium – Polypyridine complexes with aromatic ami 	nes"(5)
ii) Explain the format for the journal, tetrahedron and differentiate the s	
from that of Indian Journal of Chemistry.	(5)
8. (a) i) Write short notes on multiple linear regression.	(5)
ii) What is meant by correlation coefficient? How is it calculated? Discrete	
importance	(5)
(or)	
(b) i) Write down the differences between precision and accuracy.	(4)
ii) Explain the normal distribution of random errors.	(6)
9. (a) With a neat diagram explain the basic organization of a computer.	
(or)	
(b) Write a short note on the following i) W W W	(5)
ii) Online search of chemistry databases.	(5)
ii) Online scarcii of chemistry databases.	(5)
10. (a) Explain with an example the data types supported by C language.	(3)
(or)	
(b) Write a short note on the following	
i) While	(3)
ii) While-do	(3)
iii) for	(4)

Model Question Paper

M.Phil., Degree – Branch IV (M) Chemistry (For the candidates admitted from 2012-2013 onwards)

SPECTROSCOPIC AND INSTRUMENTAL METHODS IN CHEMICAL INVESTIGATIONS

Time: Three Hours Maximum: 75 marks

Part - A (5x5=25 marks) Answer All Questions All questions carry equal marks

1. (a) Discuss the principle of spin decoupling technique in ¹H NMR spectroscopy.

(b) What is meant by Hyperfine splitting? How is it used in the predictions of

2. (a) Write a short note on Doppler effect.

- (b) Discuss Mc Lafferty Rearrangement.
- 3. (a) Define life time (Ť) of a fluorophore.

(or)

(b) Explain how Fermi Resonance is used in the prediction of frequencies in IR spectroscopy.

(or)

4. (a) Discuss Zeeman effect.

ESR results?

(or)

- (b) Discuss the excitation and ejection process in PES.
- 5. (a) What are the two parameters derived from polarograms? Explain their significances.

(or)

(b) Give the theoretical principles of electrogravimetry

Part-B (5x10=50 Marks) **Answer All Questions**

(a) Discuss the principle of ¹³C NMR and explain how the peak assignments are made. (10)

(or)

- (b) Predict the ESR spectra of the Naphthalene radical anion, Pyrazine anion radical and Cyclopentadienyl radical and discuss.
- 7. (a) Discuss how the Mossbauer spectroscopy is used to study the spin states of Complexes.

(or)

- (b) How could the following pairs of isomeric compounds be differentiated by mass spectrometry?
 - i) 2- pentanol and 2- methyl butan-2-ol.
 - ii) n –propyl cyclohexane and 1,2,4-trimethyl cyclohexane.
- 8. (a) i) State whether the following pairs of compounds can be distinguished by their IR spectra. (2x2=4)
 - (A) C_6H_5 -NH₂ and $(C_6H_5)_2$ NH
 - (B) H₂N-C₆H₄-CO₂ Me and Me-C₆H₄-CONH₂
 - (ii) What is Raman Effect? Give an account on the applications of it. (6) (or)
 - (b) Discuss the theory, instrumentation and applications of FTIR spectroscopy.
- 9. (a) (i) How will you ascertain the structure and orientation of a compound using XRD?

(or)

- (b) Discuss the theory of AAS and enumerate its applications
- 10. (a) How are amperometric titrations carried out? Discuss the principles involved. Give their merits and demerits.

(or)

(b) (i) Discuss the theory and applications of cyclic voltammetry.
