# **M.Phil. CHEMISTRY**

SEM	COURSE CODE	COURSE	CC	DURSE TITLE	NO. OF HOURS	CREDIT	CIA MARKS	SE MARKS	TOTAL MARKS
I	14MPCH1C1	CORE - I	Research Methodology in Chemistry		4*	4	40	60	100
	14MPCH1C2	CORE - II	Physical Methods in Chemistry		4*	4	40	60	100
	14MPCH1C3	CORE-III	Research Topics in Chemistry		4*	4	40	60	100
	14MPCH1C4	CORE -IV	Teaching Methodology		4*	4	40	60	100
*One hour library for each course									
TOTAL					16	16	160	240	400
II	14MPCH2PW	PROJECT WORK		Dissertation**	-	8	-	-	200
GRAND TOTAL						24	-	-	600

<sup>\*\* (</sup>Evaluation of the Dissertation shall be made jointly by the Research Supervisor and the External Examiner)

# Project (M.Phil)

Maximum Marks: 200

I review 20 Marks
II review 20 Marks
Evaluation of project 120 Marks
Viva voce 40 Marks

#### **SEMESTER -I: CORE - I**

#### RESEARCH METHODOLOGY IN CHEMISTRY

Course Code: 14MPCH1C1 Max. Marks: 100
Hours/Week: 4 Internal Marks: 40
Credit: 4 External Marks: 60

#### **Objectives:**

- > To understand the principles of research, literature survey and writing research paper and thesis writing.
- ➤ To study the statistical analysis of data, C and C++ programming.

## Unit - I Principles of Research

12 hours

12 hours

Definition - Need for research. Objectives - Motivation - Types of research - Significance - Formulation of Research Problem - Developing Hypothesis - Preparing Research Design - Selection of Research Problem - Determining Sample Design Characteristics of a Good Sample Design - Collection of Data - Methods of Data Collection - Execution of Work. Analysis of Data - Hypothesis, Testing - Generalization and Interpretation - Preparation of Report - \*Submission of Report in the form of Thesis \*.

## Unit - II Survey of Literature

Need for literature survey – Primary, Secondary and Tertiary Sources. Journals, Chemical Abstracts – Subject index, Substance index, Author index, Formula index and other indices. Other similar abstracts for special topics. Current Titles – Reviews – Monographs – Selection of Research topic – Selection of Research Facility – Location of Journals and Articles. Use of computers in the Literature Survey – Websites – Search Engines - chemspider, google scholar, scifinder, scopus, Internet, E-mail. \*Scientific Information and Documentation Centers – INSDOC, BANSDOC, NCSI, British Library – Digital Library – e-Journals – e-Content \*.

# Unit - III Assignment, Research Paper and Thesis Writing 12 hours

Assignment – Topic selection, Front Page, Text and References. Research Paper – Preparation of Manuscript for Publication in International Journals Published by Elsevier, Interscience, Wiley and Springer. Submission Procedure.

Thesis - Rough drafting - Title, Abstract, Introduction, Scope of the Work, Literature Review, Problem and Time Limitation, Experimental Methods, Results and Discussion Foot Notes. Data Presentation - Figures and Tables. Sign Conventions followed. Bibliography - Conclusion and Recommendations. Abbreviations used. \*Storing and Retrieval of Information using Computer - CD, Pen Drive, DVD \*.

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 – V C and C<sup>++</sup> Programming 12 hours

Fundamentals of C – Character set – identifiers – keywords – data types – Constants – Variables – symbolic constants – operators – expressions – evaluation of expressions. Input and Output functions – get char – put char – scanf – Printf – gets and puts functions. Control Statements – if, if-else, nesting of if-else, Switch case and break statements. Looping Statements: while, do-while, for and go to Statements. Arrays – one dimensional, two dimensional and multi dimensional arrays – pointers – Structures and union. Functions – need for defined function -Category of Functions – call by value and call by reference – recursion – #File management in C #.

# **C**<sup>++</sup> **Programming**

Object oriented programming - principles, Classes - Examples and structure. Declarations, reference arguments, arguments by value, Constructors and destructors. Virtual functions, Inheritance (Simple examples only). Overloading (Simple examples), #file handling techniques #.

# #\_\_\_\_\_# Self study

#### **TEXT BOOKS:**

- 1. Research Methodology (Methods & Techniques) , C.R. Kothari. 2<sup>nd</sup> Edn., Wishwa Prakasam,2002.
- 2. Analytical Chemistry, Scoog, West, Holler and Crouch. Thomson India 8<sup>th</sup> Edn., 2007.
- 3. Programming in C ANSI C by E. Balagurusamy, 2<sup>nd</sup> edition Tata McGraw Hill, 2001.
- 4. Programming in  $C^{++}$  Ansi C by E.Balagurusamy  $2^{nd}$  edition Tata McGraw Hill, 2001.

UNIT I : Text Book 1 UNIT II : Text Book 1 UNIT III : Text Book 1 UNIT IV : Text Book 2 UNIT V : Text Book 3,4

## **REFERENCES:**

- 1. Thesis and Assignment writing, J. Anderson, B.H.Durston and M.Poole, John Wiley Publications, Sydney. 1970.
- 2. How to write a research paper, R.Berry, Pergoman, 1969.
- 3. Computers in Chemistry, K.V. Raman, Tata McGraw-Hill Publishing company Limited, New Delhi, 2005.
- 4. Analytical Chemistry ( Theory and Practice) by R.M. Verma. CBS Publishers and Distributers, 2001.

#### **SEMESTER -I: CORE - II**

#### PHYSICAL METHODS IN CHEMISTRY

Course Code : 14MPCH1C2 Max. Marks : 100
Hours/Week : 4 Internal Marks : 40
Credit : 4 External Marks : 60

## **Objectives:**

- > To study the applications of UV- Vis, IR, Raman, <sup>1</sup>H NMR, <sup>13</sup>C NMR and mass spectroscopy
- > To study the application of computer modeling
- ➤ To understand the X-ray, neutron and electron diffraction studies

Unit – I 12 hours

Combined applications of UV- Vis, IR and Raman,  $^{1}H$  NMR,  $^{13}C$  NMR and mass spectral data for solving the structure of organic molecules, applications of NMR study relevant to stereochemistry of organic molecules. Calculation of  $\lambda$ -max for conjugated systems and carbonyl compounds,  $^{*}Application$  of UV-Vis to study geometrical isomers  $^{*}$ , Calculation of hydrogen index.

Unit – II 12 hours

Combined applications of UV-Vis, IR, <sup>1</sup>H NMR and EPR spectral data for solving the structure of metal complexes. Calculation of g-value for Cu<sup>2+</sup>,Mn<sup>2+</sup>,Co<sup>2+</sup> and Ni<sup>2+</sup> and to establish geometry of the complexes. <sup>#</sup>Application of UV – Visible to study geometry of the complexes. <sup>#</sup>.

### **Unit – III : Computational Chemistry**

12 hours

**Molecular Modeling:** Introduction – Coordinate Systems – Potential Energy surfaces-Molecular graphics – Surfaces – Mathematical concepts-molecular mechanics. Introduction to non-bonded interactions – electrostatic interactions – van der Waals interactions – Many-body effects in empirical potentials – effective pair potentials – hydrogen bonding in molecular mechanics – force field models for the simulation of liquid water.

**\*Computer simulation methods:** Introduction – calculation of simple thermodynamic properties – phase space – practical aspects of computer simulation\*.

#### **Unit- IV: Application of XRD studies in structural analysis**

12 hours

**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 – Relationship between molecular symmetry and crystallographic symmetry – basic concepts and examples. Concept of reciprocal lattice and its application – X –ray diffraction by single crystals – structure factor – determination of space group by heavy atom method – Fourier synthesis – refinement of structure.

**Neutron diffraction** – magnetic scattering – application and comparison with X- ray diffraction.

**Electron diffraction** – basic principles and applications to simple molecules.

Unit – V 12 hours

Principles and applications of special techniques such as SEM, TEM, AFM and AAS.

**Electro analytical techniques :** Polarography – Principle, factors affecting limiting current, Ilkovic equation, Half wave Potential, Instrumentation, Polarographic analysis, Evaluation of Polarographic waves, \*\*applications of polarography\*\*.

#\_\_\_\_\_# Self study

#### **TEXT BOOKS:**

- 1. P.S. Kalsi "Spectroscopy of Organic Compounds", 6<sup>st</sup> Ed., New Age International Publishers. 2004.
- 2. R.S. Drago "Physical Methods in Chemistry", W.B. Sounders.
- 3. Andrew R. Leach, Molecular Modelling second edition Pearson Prentice Hall, England 2001.
- 4. Grudeep.R.Chatwal, Sham. K Anand Instrumental methods of chemical analysis, Himalaya publishing house pvt ltd., Mumbai reprint- 2008.
- 5. H.Kaur, Instrumental methods of chemical analysis, Pragati prakasan, Meerut 2006.
- 6. P.S. Kalsi "Spectroscopy of Organic Compounds", 6<sup>st</sup> Ed., New Age International Publishers. 2004.

UNIT I : Text Book 1,6 UNIT II : Text Book 2 UNIT III : Text Book 3 UNIT IV : Text Book 4 UNIT V : Text Book 5

#### **REFERENCES:**

- 1. B.P. Straughan and S. Walker "Spectroscopy", Vol. 1, Chapman and Hall 1967.
- 2. H. Kaur "Spectroscopy", 3<sup>rd</sup> Ed., Pragati Prakasan Publications, Meerut, 2006.
- 3. E.A.V. Ebsworth, W.H. Rankin, Cradock "Structural Methods in Inorganic Chemistry", ELBS, 1987.
- 4. Robert M. Silverstein, Francis X. Webster, David Kiemle "Spectrometric Identification of Organic Compounds", John Wiley & sons (2005).
- 5. A.K.Srivastava and P.C. Jain, Instrumental approach to chemical analysis, S.chand company ltd. Fourth revised edition-2009.
- 6. Willard, Merrit, Dean and Settle, "Instrumental Methods of Analysis" CBS Publishers and Distibutors, 6<sup>th</sup> ed., 1986.

# SEMESTER -I: CORE - IV TEACHING METHODOLOGY

Course Code : 14MPCH1C4 Max. Marks : 100
Hours/Week : 4 Internal Marks : 40
Credit : 4 External Marks : 60

## **Objectives:**

> To study the computer application, communication and education skill

To study the teaching strategies and education technology

# Unit – I Computer Application Skill

12 hours

Internet – meaning – importance – types of networking – LAN, WAN, MAN – Internet – WWW, website and webpage's, Internet connectively – Browsing the internet – Browsing software – URL addresses, search engines, exploring websites and downloading materials from websites, E-mail – sending, receiving and storing mail and chatting. Power point – creating a presentation – slide preparation – popular websites for data collection in chemistry.

## **Unit - II Communication and Interaction**

12 hours

The theory of communication – communication cycle – Types of communication, communication and language, communication in the class room, Lecture and Lecture demonstration as communication. Interaction methods – Interaction analysis, observation schedule and record. Bale's interaction process categories – Flander's system of interaction analysis – verbal interaction category system. \*Reciprocal category system – Equivalent talk categories\*.

#### Unit – III Educative Skill 12 hours

Psychology – Definition – Nature – Meaning of Educational Psychology – Definition – Nature – Scope. Teaching and learning – meaning – characteristics –effective teaching – concept of learning –comparison between teaching and learning. Mental health – Frustration – concept of adjustment – Defence mechanism – Mental hygiene.

# Unit – IV Uses of teaching strategies

12 hours

Group methods of instruction – lecture – demonstration – seminars – workshops – case analysis – panel discussion – team teaching – individual approaches – Teleconferencing – Video conferencing – Description – Advantages – Micro teaching – Characteristics of Micro teaching – Teaching skills - Programmed Instruction - Computer Assisted Instruction (CAI) – \*Language Laboratory\*.

Educational technology – definition – objectives – teaching technology – characteristics of teaching technology – behavioural technology – pedagogy of teaching – General advantage of using teaching aids – Broad classification of teaching aids – Hardware and software in teaching aids. Instructional media – media attributes – multimedia and instructional development – \*Multimedia centre – uses and abuses of multimedia\*.

#\_\_\_\_\_# Self study

#### **TEXT BOOKS:**

- 1. Zikr ur Rahman, Modern teaching methods and techniques, Anmol Publication Pvt. Ltd. New Delhi, (2006).
- 2. R.A.Sharma, Educational technology and management models media and methods, R. Lall Book Depot. Meerut, (2007).
- 3. Vanaja, Educational technology –, Neel Kamal publications Pvt. Ltd. Hyderabad, (2004).

UNIT I : Text Book 1 UNIT II : Text Book 2,3 UNIT III : Text Book 2,3 UNIT IV : Text Book 2,3 UNIT V : Text Book 2,3

#### **References:**

- 1. B.N. Dash, Elementary Educational Psychology and Methods of teaching, Neel Kamal publications Pvt. Ltd., New Delhi, (2004 and 2007).
- 2. P. Sambasiva Rao and D. Bhaskar Rao, Techniques of Teaching Psychology, Sonali publications New Delhi, (2006).
- 3. S. K. Kochhar, Methods and Techniques of Teaching, Sterling Publisher Pvt. Ltd. (2004).
- 4. K. Sampath, A. Panner selvam and S. Santhanam, Introduction to Educational Technology, 4<sup>th</sup> revised ed., Sterling Publisher Pvt. Ltd (2000).
- 5. S. Robinson, Fundamentals of Education Psychology, 2<sup>nd</sup> ed., Ane Books Pvt. Ltd, (2008).
- 6. T.M. Srinivasan, Use of Computers and Multimedia in Education, Aavisakar publication, Jaipur (2002).
- 7. K. Sundarrajan, Internet, Kannadhasan publications, Chennai (1998).