

**MOTHER TERESA WOMEN'S UNIVERSITY**

**KODAIKANAL – 624 101**

**M.Phil. DEGREE COURSE IN CHEMISTRY**

**(For candidates admitted from the academic year 2021-2022 onwards)**



**DEPARTMENT OF CHEMISTRY**

**MOTHER TERESA WOMEN'S UNIVERSITY, KODAIKANAL**

## **M.Phil. CHEMISTRY SYLLABUS**

### **1. Objectives:**

1. To introduce and provide knowledge of research methodology.
2. To provide a sound knowledge in the advanced concepts of chemistry.
3. To impart research aptitude and provide adequate training in synthesis, characterization instrumentation
4. To provide an exposure to research

### **2. Eligibility for Admission**

A candidate who has secured 50% marks or above in the M. Sc. Chemistry degree examination shall be eligible for admission.

The duration of the course shall be for two academic years consisting of four semesters

### **3. Course Features**

The M. Phil. Chemistry degree course comprises of four theory papers. The paper Professional skills is common for all the courses.

The duration of the course shall be for one academic year consisting of two semesters

The paper on the topic of research concerns with the area of specialization chosen by the candidate under a guide which will be related to the project work. It is purely internal (Syllabus framing and question setting)

Each candidate will submit a dissertation on a topic in chemistry after carrying a research project under the supervision of the guide. The duration of the project will be for six months or more as per the discretion of the Department. The project dissertation will be evaluated by an external examiner and viva voce will be conducted by a committee consisting of the guide and the department faculty.

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KODAIKANAL  
M.Phil. CHEMISTRY**

S. No	Code	Subject	Hours	Credits	Internal	External	Total
<b>First Semester</b>							
1	M21CHT11	Research Methodology	10	4	40	60	100
2	M21CHT12	Advances in Chemistry	10	4	40	60	100
3	M21PST13	Professional skills	10	4	40	60	100
			30	12			300
<b>Second Semester</b>							
4	M21CHT21	Special Paper related to Project	10	4	40	60	100
5	M21CHD21	Dissertation+ Viva Voce	20	14(12+2)	120	80	200
			30	18			300
				<b>30</b>			<b>600</b>

**Special papers related to Project**

S. No	Title
1.	Coordination Chemistry and Spectroscopy
2.	Crystallography & Supramolecular Chemistry
3.	Directed Study*

\*Any new course can be added as a special paper by getting permission from BOS and Academic Council

## SEMESTER I

### PAPER I

**MCHT11**

**RESEARCH METHODOLOGY**

**6 hours /4 credits**

#### **Objectives**

1. To introduce the purpose and importance of research
2. To impart knowledge in the various methods of research.
3. To learn the scientific method of collecting data and to compute statistical parameters to arrive at meaningful conclusions.
4. To know the methodology of writing thesis and journal articles.

#### **Unit I : Philosophy of Science and literature survey**

Literature survey – Sources of information – Primary, Secondary, Tertiary sources – Chemical Journals – Journal abbreviations. Chemical abstracts – Subject Index, Author Index, Formula Index and other Indices with examples. Dictionary of Compounds – Beilsteins and other hand books

Web resources – E-Journal – Citation index – Impact factor – H-Index – E-Consortium – UGC infonet – E-Books – Search engines: Scirus, Google Scholar, Chem Industry, Wiki – Databases: Chem Spider, Science Direct, SciFinder, Scopus

#### **Unit II : Methodology of Scientific Document Writing**

Introduction to technical writing-types of report, title and abstract, the text-style and conventions in writing. Writing dissertation and thesis – Title, Abstract, Introduction, Literature Review, Experimental Methods, Results and Discussion, Foot notes, Figures, Data Presentation, Tables, Sign Conventions followed – Conclusions and Recommendations – Bibliography.

Preparation of manuscript and posters – writing review article and book reviews – preparing research proposals for grants – ethics in scientific publication – formats for some national and international journals.

#### **Unit III : Data Analysis**

True value - standard value - observed value – Error – Types of Errors – Accuracy – Precision, Error Analysis, Minimization of Errors, Deviation from Accurate Results - the Binomial Distribution – the Gaussian Distribution – Mean - - Median – Deviation – from Mean and Median – student’s t-test, F-test – Significant figures in multiplication – Division – Addition and Subtraction – Curve Fitting method of Least Squares – Linear Regression – Multiple Linear Regression – Slope – Intercept and Correlation Coefficient

#### **Unit IV: Chemical Safety and Ethical Handling of Chemicals**

Safe working procedure and protective environment, protective apparel, emergency procedure and first aid, laboratory ventilation, Safe storage and use of hazardous chemicals, procedure for working with substances that pose hazards, flammable or explosive hazards, procedures for working with gases at above or below atmospheric pressures – safe storage and disposal of waste chemicals , recovery , recycling and reuse of laboratory chemicals, procedure for laboratory disposal of explosives , identification , verification and segregation of laboratory waste , disposal of chemicals in the sanitary sewage system , incineration and transportation of hazardous chemicals .

#### **Unit V : Analytical techniques and Computer Packages**

The principle, instrumentation and applications of TGA/ DTA/DSC, SEM &TEM, AAS techniques.

Applications of some computer packages like MS–Excel, Origin, ChemDraw, Sciplot, ISIS draw, ChemSketch and SPSS.

#### **References**

##### **UNIT I**

1. R. L. Dominoswki, Research Methods, Prentice Hall, 1981.
2. 2. J. W.Best, Research in Education, 4th ed. Prentice Hall of India, New Delhi, 1981.

##### **UNIT II**

1. M. Coghill and L. R. Gardson, The ACS Style Guide – Effective Communication of Scientific information, 3<sup>rd</sup> Edn, Oxford University Press, 2006.
2. H. Beall and J. Trimbur, A short Guide to Writing about Chemistry, 2<sup>nd</sup> Edn, Longman, 2001.
3. J. Anderson, B.H. Durston and M.Poole, “Thesis and Assignment Writing”, John Wiley, Sydney 1970.
4. R. Berry, “How to Write a Research Paper”, Pergamon, Oxford, 1986.

5. Ralph Berry, "The Research Project: How to Write It", 4<sup>th</sup> Ed., Routledge, Taylor and Francis, London, 2000.
6. W.G. Campbell – "Form and Style in thesis Writing, Houghton Mifflin Co., Boston M.A, 1970.

### **UNIT III**

1. S. P. Gupta, Statistical Methods, Sultan Chand & Sons, New Delhi, 1993.
2. D. Brynn Hibbert and J. Justin Gooding, Data Analysis, Oxford University Press, New York, 2006.
3. C. R. Kothari, Research Methodolgy, Methods and Techniques, Wiley Eastern Ltd, New Delhi, 1991.

### **UNIT IV**

1. Handbook Good Laboratory Practice (GLP) Quality Practices for Regulated Non-Clinical Research and Development
2. Willa Y. Garner, Maureen S. Barge, and James. P, Good Laboratory Practice Standards: Applications for Field and Laboratory Studies (ACS Professional Reference Book)
3. Chemical safety matters-IUPAC –IPCS, Cambridge Univ. Press, 1992.

### **UNIT V**

1. G. D.Christian & J. E. O'Reily, Instrumental Analysis, 2nd Ed., Allyn & Balon, 1986.
2. H. H. Willard, L. L. Merritt, J. A. Dean and F. A. Settle, Instrumental Methods of analysis, 7<sup>th</sup> ed., CBS publishers, New Delhi,1986.
3. D. A. Skoog, F. J. Holler and T.M. Niemann, Principles of Instrumental Analysis, 5<sup>th</sup> Ed., Harcourt Asia Pvt. Lts.,2001
4. Srivastava, Chemical Analysis: An instrumental Approach, S. Chand, New Delhi
5. F. A. Settle,Ed. Handbook of Instrumental Technique for Analytical Chemistry, Pearson Edn., India,1997.
6. C. N. R. Rao, A. Muller, A. cheethan, Eds. The chemistry of Nanomaterials, Wiley, New York, 2004.
7. D. L. Feldheim, C. A. Fross, Jr. Metal Nanoparticles: Synthesis, Characterisation and Applications; Dekker; New York, 2002.
8. G.L.Hornyak, J.Dutta, H.F.Tibbals, A.K.Rao, Introduction to Nanoscience, CRC Press, 2008.

**Paper II****MCHT12****ADVANCES IN CHEMISTRY****6 hours /4 credits****Objectives**

1. To impart knowledge and understanding in the advanced concepts of organic chemistry
2. To impart knowledge and understanding in the advanced concepts of inorganic chemistry
3. To impart knowledge and understanding in the advanced concepts of physical chemistry
4. To impart research aptitude and provide adequate training in synthesis, characterization, instrumentation

**Unit I : Advanced Organic Chemistry**

**Organic Synthesis** - Synthetic planning, Retrosynthetic analysis and disconnection method, Functional group protection.

**Asymmetric Synthesis** - Basic principles, Asymmetric synthesis using chiral reagents, Asymmetric catalysis, catalytic asymmetric alkylation, hydrogenation, reactions catalysed by enzymes and other proteins. Organo transition metal chemistry-Applications to asymmetric synthesis.

**Green Chemistry** –Twelve principles of green chemistry - Green chemical methods of synthesis-use of microwaves in organic synthesis - solventless reactions - green solvents - supercritical fluids for extraction - ionic liquids

**Unit II : Advanced Physical Chemistry****Electrochemical Techniques & computational Chemistry**

Principles of polarization techniques, Principles of voltammetry, cyclic voltammetry.

Computational Chemistry: *Ab initio*, DFT and semi-empirical methods-Energy minimization; Local and global energy minima, saddle point-Electronic descriptors-Force fields-Monto Carlo simulation-QSAR-Regression methods-Function modules of molecular softwares.

Molecular docking- Molecular Dynamics; Introduction, basic principles, conformation analysis, Mechanics and dynamics of Bio-macromolecules.

### **Unit III: Advanced Inorganic Chemistry**

**Spectral and Magnetic properties of complexes:** Electronic spectra of metal complexes, selection rules, term symbols, correlation diagrams - electronic spectra of  $d^n$  ions, Magnetic susceptibility, application of magnetic moments to structure elucidation of metal complexes.

**Medicinal Inorganic Chemistry:** Contrast enhancing agents for medical diagnostics, theory of MRI imaging, Gd based contrast agents-synthesis and structural features; optical contrast agents- Ag and AuNPs. Metal complexes for radiotherapy, diagnostic radiopharmaceuticals. Applications of organometallics in medicine and industries

### **Unit IV ; Spectroscopy I**

#### **Nuclear Magnetic Resonance Spectroscopy**

**$^1\text{H}$  NMR spectroscopy :** Chemical shift – number of signals – peak areas – multiplicity – geminal, vicinal and long – range couplings – factors affecting these parameters

**$^{13}\text{C}$ NMR spectroscopy:** Broadband of off-resonance decoupling, comparison of  $^1\text{H}$  and  $^{13}\text{C}$ NMR – factors affecting intensity of signals – chemical shifts -  $\gamma$  - gauche effect

**2D NMR:** NOESY and COSY, application of  $^1\text{H}$  NMR &  $^{13}\text{C}$  NMR in structure elucidation

**Mass spectroscopy** - basic principles – molecular ion peak, parent peak, fragments, metastable peak, isotope peaks – determination of molecular weight and molecular fragment – fragment pattern of simple organic molecules – McLafferty rearrangement

### **Unit V : Spectroscopy II**

**ESR spectroscopy** – Basic concepts- Factors affecting the magnitude of  $g$  and  $A$  tensors in metal complexes – Anisotropy in  $g$  and  $A$  values - Zero-field splitting and Kramers degeneracy - Applications of EPR to  $\text{Cu(II)}$ ,  $\text{Fe(II)}$ ,  $\text{Mn(II)}$  and  $\text{Ni(II)}$  complexes.

Combined spectroscopy problems involving IR, UV, Mass and NMR.

### **Reference Books**

#### **Unit I**



1. R.E.Ireland, Organic Synthesis, Prentice Hall, 1969.
2. S.Turner, Design of Organic Synthesis, Elsevier, 1976.
3. S.Warren, Designing Organic Synthesis – A programmed introduction to synthon approach, Wiley, New York, 1978.
4. R.T. Morrison and R.N. Boyd, Organic Chemistry, 6<sup>th</sup> Ed., Pearson, 1992.
5. J.March, Advanced Organic Chemistry, 4<sup>th</sup> Edn. John Wiley, New York, 1992

### **Unit II**

1. Joseph R.Lakowicz “Principle of Fluorescence Spectroscopy” Third Edn. Springer, USA, 2006
2. A. Sharme, S. G. Schulman, Introduction to Fluorescence Spectroscopy, John Wiley & Sons, Inc., New York, 1999.
3. H. Kissinger, Electroanalytical Techniques, John Wiley, 1998

### **Unit III**

1. J.E. Huheey, Inorganic Chemistry, 3<sup>rd</sup>. Ed., Harper & Row publisher, 1983.
2. D.E. Douglas, D.H. McDaniel, J.J. Alexander, Concepts and Models in Inorganic Chemistry, 3<sup>rd</sup> Ed. 1994.
3. J.D. Lee, Concise Inorganic Chemistry, 5<sup>th</sup> Ed, Wiley, 1999.
4. E.A.V. Ebsworth, Structural Methods in Inorganic Chemistry, 3<sup>rd</sup> Ed., ELBS, 1987
5. C E Coates. M L H Green, P Powell K Wade Principles of Organometallic Compounds, Chapman and Hall, 1977.
6. M. F. Purcell, J. C. Kotz, Inorganic Chemistry, Saunder, 1977.

### **Unit IV**

1. P.M. Silverstein, F.X. Wester, Spectroscopic Identification of Organic Compounds, 6<sup>th</sup> Ed., Wiley 1998.
2. Mohan, Organic Spectroscopy Principles and Applications, 2<sup>nd</sup> Ed., CRC, 2004.
3. Kemp, Organic Spectroscopy, 3<sup>rd</sup> Ed., MacMillon, 1994.
4. L. Pavia, G.M. Lampman, G.S. Kriz, Introduction to Spectroscopy, 3<sup>rd</sup> Ed., Brooks Cole, 2000.

### **Unit V**

1. E.A.V. Ebsworth, Structural Methods in Inorganic Chemistry, 3<sup>rd</sup> Ed., ELBS, 1987.
2. R.S. Drago, Physical Methods in Inorganic Chemistry, 3<sup>rd</sup> Ed., Wiley Eastern Company
3. R.S. Drago, Physical Methods in Chemistry, W. B. Saunders Company, 1992.
4. J.E. Huheey, Inorganic Chemistry, 3<sup>rd</sup>. Ed., Harper & Row publisher, 1983.
5. D.E. Douglas, D.H. McDaniel, J.J. Alexander, Concepts and Models in Inorganic Chemistry, 3<sup>rd</sup> Ed. 1994.
6. P.M. Silverstein, F.X. Wester, Spectroscopic Identification of Organic Compounds, 6<sup>th</sup> Ed., Wiley 1998.

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