



**V.V.VANNIAPERUMAL COLLEGE FOR WOMEN**  
 (Belonging to Virudhunagar Hindu Nadars)  
 An Autonomous Institution Affiliated to Madurai Kamaraj University, Madurai  
 Re-accredited with 'A' Grade (3<sup>rd</sup> Cycle) by NAAC  
**VIRUDHUNAGAR - 626 001**

**OUTCOME BASED EDUCATION WITH CHOICE BASED CREDIT SYSTEM  
 REGULATIONS AND SYLLABUS  
 (with effect from Academic Year 2020 - 2021)**

V.V.Vanniaperumal College for Women, Virudhunagar, established in 1962, offers 20 UG Programmes, 14 PG Programmes, 6 M.Phil. Programmes and 6 Ph.D. Programmes. The curricula for all these Programmes, except Ph.D. Programmes, have been framed as per the guidelines given by the University Grants Commission (UGC) & Tamil Nadu State Council for Higher Education (TANSICHE) under Choice Based Credit System (CBCS) and the guidelines for Outcome Based Education (OBE).

The Departments of Commerce, English, History, Mathematics, Biochemistry and Tamil upgraded as Research Centres offer Ph.D. Programmes as per the norms and regulations of Madurai Kamaraj University, Madurai and do not come under the purview of CBCS.

**A. CHOICE BASED CREDIT SYSTEM (CBCS)**

The CBCS provides an opportunity for the students to choose courses from the prescribed Courses. The CBCS is followed as per the guidelines formulated by the UGC. The performance of students is evaluated based on the uniform grading system. Computation of the Cumulative Grade Point Average (CGPA) is made to ensure uniformity in evaluation system.

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**List of Programmes in which CBCS/Elective Course System is implemented**

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**UG PROGRAMMES**

Arts & Humanities	: History (E.M. & T.M.), English, Tamil
Physical & Life Sciences	: Mathematics, Zoology, Chemistry, Physics, Biochemistry, Home Science - Nutrition and Dietetics, Costume Design and Fashion, Microbiology, Biotechnology, Computer Science, Information Technology and Computer Applications.
Commerce & Management	: Commerce, Commerce (Computer Applications), Commerce (Professional Accounting), Business Administration.

**PG PROGRAMMES**

Arts & Humanities	: History, English, Tamil
Physical & Life Sciences	: Mathematics, Physics, Biochemistry, Home Science - Nutrition and Dietetics, Chemistry, Zoology, Computer Science, Information Technology, Computer Applications (MCA*)
Commerce & Management	: Commerce, Business Administration (MBA*) * AICTE approved Programmes

**PRE-DOCTORAL PROGRAMMES (M.Phil.)**

Arts & Humanities	: History, English, Tamil
Physical & Life Sciences	: Mathematics, Biochemistry
Commerce & Management	: Commerce

**OUTLINE OF CHOICE BASED CREDIT SYSTEM - PG**

1. Core Courses
2. Practical
3. Project
4. Elective Courses
  - 4.1 Discipline Specific Elective Courses (DSEC)
  - 4.2 Non Major Elective Course (NMEC)
5. Online Course – Practice for CSIR NET – General Paper
6. Extra Credit Courses (Optional)

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**List of Non Major Elective Courses (NMEC) Offered**


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**PG PROGRAMMES**

Name of the Course	Semester	Department
History of Freedom Movement in India (A.D. 1885 - 1947)	III	History
English for Job Aspirants	III	English
jkpOk; gpwJiwfSk;	III	Tamil
Taxation Concepts and Assessment	III	Commerce
Entrepreneurship	III	Business Administration
Mathematics for Competitive Examinations	III	Mathematics
Digital Electronics	III	Physics
Chemistry for Competitive Examinations	III	Chemistry
Apiculture	III	Zoology
Nutrition and Health	III	Home Science - Nutrition and Dietetics
Clinical Biochemistry	III	Biochemistry
Web Programming	III	Computer Science
Fundamentals of Information Technology	III	Information Technology
Web Technology	III	Computer Applications

## **B. OUTCOME BASED EDUCATION (OBE) FRAMEWORK**

The core philosophy of Outcome Based Education rests in employing a student - centric learning approach to measure the performance of students based on a set of pre-determined outcomes. The significant advantage of OBE is that it enables a revamp of the curriculum based on the learning outcomes, upgrade of academic resources, quality enhancement in research and integration of technology in the teaching-learning process. It also helps in bringing clarity among students as to what is expected of them after completion of the Programme in general and the Course in particular. The OBE directs the teachers to channelise their teaching methodologies and evaluation strategies to attain the Programme Educational Objectives (PEOs) and fulfill the Vision and Mission of the Institution.

### **Vision of the Institution**

The founding vision of the Institution is to impart Quality Education to the rural womenfolk and to empower them with knowledge and leadership quality.

### **Mission of the Institution**

The mission of the Institution is to impart liberal education committed to quality and excellence. Its quest is to mould learners into globally competent individuals instilling in them life-oriented skills, personal integrity, leadership qualities and service mindedness.

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### **B.1 Programme Educational Objectives, Programme Outcomes and Programme Specific Outcomes**

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It is imperative for the Institution to set the Programme Educational Objectives (PEOs), Programme Outcomes (POs) and Course Outcomes (COs), consistent with its Vision and Mission statements. The PEOs and the POs should be driven by the Mission of the Institution and should provide distinctive paths to achieve the stated goals. The PEOs for each Programme have to fulfill the Vision and Mission of the Department offering the Programme.

### **Vision of the Department of Chemistry**

To train our students as scientifically literate professionals with a sense of social responsibilities.

### **Mission of the Department of Chemistry**

- To provide advanced knowledge in chemistry.

- To develop in students employable skills for job opportunities in the field of education, R&D institutions and industries.
- Acquire knowledge, abilities and insight in well-defined area of research within Chemistry.
- Acquire the skills of planning and conducting advanced chemical experiments and applying structural-chemical characterization techniques.
- Examine specific phenomena theoretically and/or experimentally, contribute to the generation of new scientific insights or to the innovation of new applications of research in Chemistry.

### B.1.1 Programme Educational Objectives (PEOs)

PEOs are broad statements that describe the career and professional achievements that the Programme is preparing the graduates to achieve within the first few years after graduation. PEOs are framed for each Programme and should be consistent with the Mission of the Institution.

#### Programme Educational Objectives (PEOs) of M.Sc. Programme

##### The students will be able to

- To educate and guide the students in attaining significant opportunities in various service domains at national and international level, and can work as scientist, analyst, quality controller, academics, research organizations and set testing labs.
- To mould the overall personality of the students by providing training and opportunities to enhance their communication skills, team management, co-ordination skills and leadership qualities.
- To guide and create awareness among the students to learn and adopt new skills and techniques to overcome the problem related with new technologies and to formulate, investigate and analyze scientifically real life problems along with ethical attitude which works in multidisciplinary team.

Key Components of the Mission Statement	PEO1	PEO2	PEO3
advanced knowledge and practical experience	√	-	√
development of research activities among students	√	√	√
employable skills for job opportunities	√	√	√
Contributing innovation of new applications of research in chemistry.	√	-	√

## 1.2 Programme Outcomes (POs)

POs shall be based on Graduate Attributes (GAs) of the Programme. The GAs are the attributes expected of a graduate from a Programme in terms of knowledge, skills, attitude and values. The Graduate Attributes include Disciplinary Knowledge, Communication Skills, Critical Thinking, Problem Solving, Analytical Reasoning, Research Related Skills, Co-operation/Team Work, Scientific Reasoning, Reflective Thinking, Information/Digital Literacy, Multicultural Competence, Moral and Ethical Awareness/Reasoning, Leadership Qualities and Lifelong Learning.

### On successful completion of the Programme, the students will be able to

- 1 apply their in depth domain knowledge and practical skills in interdisciplinary fields for research-based endeavours, employment and entrepreneurship development. (*Disciplinary Knowledge*)
- 2 communicate proficiently and confidently with the ability to present complex ideas in a concise manner to assorted groups. (*Communication Skills*)
- 3 identify, formulate and solve problems in a consistent and systematic way with updated skills using modern tools and techniques. (*Scientific Reasoning and Problem Solving*)
- 4 analyze the data, synthesise the findings and provide valid conclusion by critical evaluation of theories, policies and practices for the betterment of society. (*Critical Thinking and Analytical Reasoning*)
- 5 explore and evaluate globally competent research methodologies to apply appropriately in interdisciplinary research; Develop and sustain the research capabilities to meet the emerging needs for the welfare of the society. (*Research Related Skills*)
- 6 use ICT to mould themselves for lifelong learning activities to face career challenges in the changing environment. (*Digital Literacy, Self - Directed and Lifelong Learning*)
- 7 self-manage and function efficiently as a member or a leader in diverse teams in a multicultural society for nation building. (*Co-operation/Team Work and Multicultural Competence*)
- 8 uphold the imbibed ethical and moral values in personal, professional and social life for sustainable environment. (*Moral and Ethical Awareness*)

### B.1.3 Programme Specific Outcomes (PSOs)

Based on the Programme Outcomes, Programme Specific Outcomes are framed for each PG Programme. Programme Specific Outcomes denote what the students would be able to do at the time of graduation. They are Programme-specific and it is mandatory that each PO should be mapped to the respective PSO.

**On successful completion of M.Sc. Programme, the students will be able to**

**PO 1: *Disciplinary Knowledge***

**PSO 1.a :** Apply in - depth knowledge on advanced concepts in Organic, Inorganic, Physical, Analytical, Biological, Environmental and Industrial applications of chemistry in research based endeavours.

**PSO 1.b :** Apply appropriate techniques for the qualitative and quantitative analysis of chemicals in laboratories and in industries.

**PO 2: *Communication Skills***

**PSO 2 :** Communicate effectively on scientific achievements, basic concepts and recent developments with experts and with society at large; comprehend and write reports, documents, make effective presentation by oral and/or written form.

**PO 3: *Scientific Reasoning and Problem Solving***

**PSO 3.a :** Develop analytical, technical and problem solving skills to handle the corrosive, poisonous, explosive and carcinogenic chemicals making themselves employable in any kind of chemical industries. Train about the adverse effects of the abnoxious chemicals and the first aid treatment.

**PSO 3.b :** Use modern chemical tools, Models, Chemdraw, Charts and Advanced Equipments for the potential uses in analytical industrial chemistry, medicinal chemistry and green chemistry.

**PO 4: *Critical Thinking and Analytical Reasoning***

**PSO 4 :** Employ critical thinking and the scientific knowledge to design, carry out, record and analyze the results of chemical reactions to create an awareness of the impact of chemistry on the environment and society.

**PO 5: *Research Related Skills***

**PSO 5 :** Come out with clear idea of choosing original research problems, writing new projects and publishing research papers to open up new methods for environmental protection, resource management, public health and safety.

**PO 6: Digital Literacy, Self - Directed and Lifelong Learning**

**PSO 6 :** Use ICT tools for literature survey of the topic of research, manuscript preparation and online submission for publication. Apply disciplinary or interdisciplinary learning across multiple contexts, integrating knowledge and equip the students to face the employment challenges and instill confidence to turn into entrepreneur.

**PO 7: Co-operation/Team Work and Multicultural Competence**

**PSO 7 :** Engage in intellectual exchange of ideas with researchers of other disciplines to address important research issues.

**PO 8: Moral and Ethical Awareness**

**PSO 8 :** Explore the impact of the solutions in ethical, societal and environmental contexts and demonstrate the knowledge of and need for sustainable development.

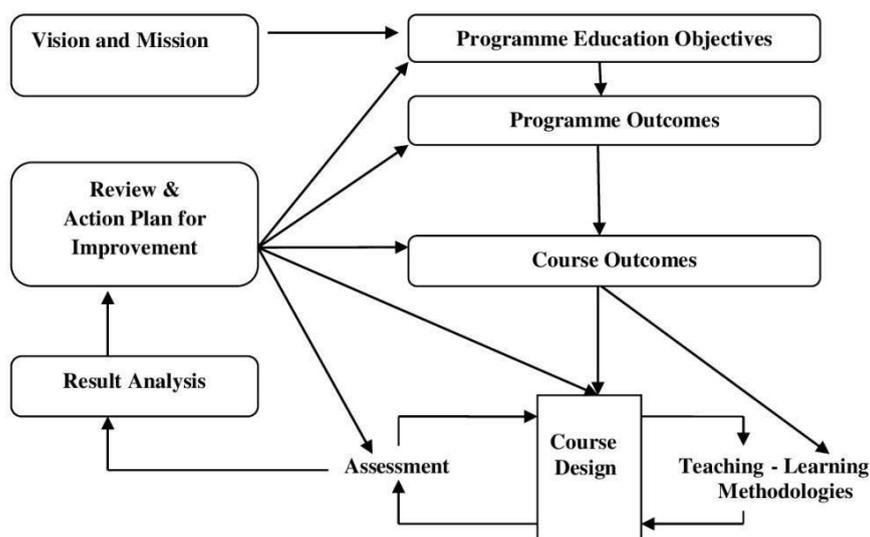
**PO-PEO Mapping Matrix**

Attainment of PEOs can be measured by a PO-PEO matrix. PEOs should evolve through constant feedback from alumnae, students, industry, management, *etc.* It is mandatory that each PEO should be mapped to at least one of the POs.

<b>POs/ PSOs</b>	<b>PEO1</b>	<b>PEO2</b>	<b>PEO3</b>
<b>PO1/PSO1</b>	√		√
<b>PO2/PSO2</b>	√	√	√
<b>PO3/PSO3</b>	√		√
<b>PO4/PSO4</b>	√	√	√
<b>PO5/PSO5</b>	√		√
<b>PO6/PSO6</b>	√	√	√
<b>PO7/PSO7</b>	√	√	√
<b>PO8/PSO8</b>	√		√

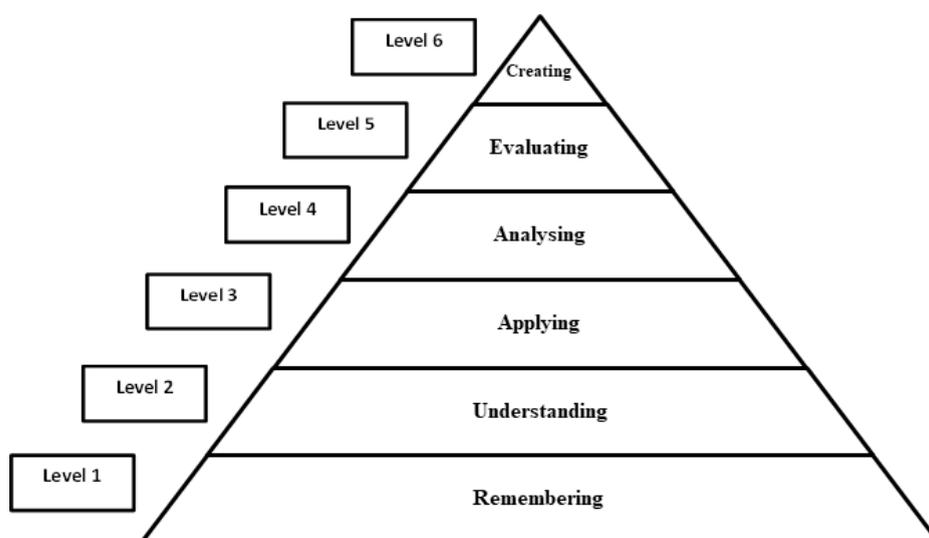
### B.1.4 Course Outcomes (COs)

Course Outcomes are narrow statements restricted to the course contents given in five units. Course Outcomes describe what students would be capable of, after learning the contents of the Course. They reflect the level of knowledge gained, skills acquired and attributes developed by the students after learning of Course contents. COs are measurable, attainable and manageable in number. COs contribute to attain POs in such a way that each CO addresses at least one of the POs and also each PO is reasonably addressed by adequate number of COs.



It is important to determine the methods of assessment. A comprehensive assessment strategy may be outlined using the revised Bloom's Taxonomy levels.

### BLOOM'S TAXONOMY



## CO - PO Mapping of Courses

After framing the CO statements, the COs framed for each course is mapped with POs based on the relationship that exists between them. The COs which are not related to any of the POs is indicated with (-), signifying Nil. Measurement Mapping is based on Four Points Scale [High (H), Medium (M), Low (L) and Nil (-)]. For calculating weighted percentage of contribution of each Course in the attainment of the respective POs, the weights assigned for H, M and L are 3, 2 and 1 respectively.

### CO-PO/PSO Mapping Table (Course Articulation Matrix)

PO/PSOs	PO1/ PSO1	PO2/ PSO2	PO3/ PSO3	PO4/ PSO4	PO5/ PSO5	PO6/ PSO6	PO7/ PSO7	PO8/ PSO8
CO1								
CO2								
CO3								
CO4								
CO5								

### ELIGIBILITY FOR ADMISSION

The candidate should have passed in B.Com. (General or any Specialisation)/ BBA/ BBM Degree from any recognized University.

### DURATION OF THE PROGRAMME

The candidates shall undergo the prescribed Programme of study for a period of two academic years (four semesters).

### MEDIUM OF INSTRUCTION

English

## B.2 EVALUATION SCHEME

Components	Internal Assessment Marks	External Examination Marks	Total Marks
Theory/Practical	40	60	<b>100</b>
Project	60	40	<b>100</b>

### B.2.1 Core Courses, Discipline Specific Elective Courses & Non Major Elective Course

#### INTERNAL ASSESSMENT

##### Distribution of Marks

##### Theory

Mode of Evaluation			Marks
Periodic Test		:	25
Assignment	K5 Level	:	5
Seminar		:	10
<b>Total</b>		<b>:</b>	<b>40</b>

Three Periodic Tests - Average of the best two will be considered

Two Assignments - Better of the two will be considered

##### Practical

Mode of Evaluation			Marks
Test		:	15
Model Examination		:	15
Performance		:	10
<b>Total</b>		<b>:</b>	<b>40</b>

Test - Average of the two will be considered

Model Examination - Better of two will be considered

Performance - Attendance and Record

#### Question Pattern for Periodic Test

**Duration: 2 Hours**

Section	Types of Question	No. of Questions	No. of Questions to be answered	Marks for each Question	Max. Marks
A Q.No.(1 - 5)	MCQ	5	5	1	5
B Q.No.(6-10)	Internal Choice - Either Or Type	5	5	5	25
C Q.No.(11-12)	Internal Choice - Either Or Type	2	2	10	20
<b>Total</b>					<b>50*</b>

\*The total marks obtained in the Periodic Test will be calculated for 25 marks

## EXTERNAL EXAMINATION

### Question Pattern

**Duration: 3 Hours**

Section	Types of Question	No. of Questions	No. of Questions to be answered	Marks for each Question	Total Marks
A Q.No.(1 - 5)	MCQ Sentence Form	5	5	1	5
B Q.No.(6-10)	Internal Choice- Either Or Type	5	5	5	25
C Q.No.(11-13)	Internal Choice - Either Or Type	3	3	10	30
<b>Total</b>					<b>60</b>

### B.2.2 Project

Project is compulsory for II PG Students in IV Semester.

#### Distribution of Marks

Mode of Evaluation		Marks
Internal Assessment	:	60
External Examination	:	40
<b>Total</b>	:	<b>100</b>

#### Evaluation Pattern (100 marks)

Internal Assessment (60marks)				External Assessment (40 marks)	
One Periodic Test (20)	Project Report (20)	Pre-Submission Presentation (10)	One Open online Course related to the Project (10)	Project Presentation (30)	Viva Voce (10)

### B.2.3 Online Course

Practice for CSIR NET - General Paper

Internal Examination only

- Online Test with Multiple Choice Questions will be conducted in III Semester.
- Model Examination will be conducted after two periodic tests.

## Distribution of Marks

Mode of Evaluation		Marks
Periodic Test	:	40
Model Examination	:	60
<b>Total</b>	<b>:</b>	<b>100</b>

Two Periodic Tests - Better of the two will be considered

### B.2.4 Extra Credit Courses

- One credit is allotted for each Extra Credit Course offered by the Department.
- Extra credits are allotted for the completion of Open Online Courses offered by MOOC to the maximum of 15 credits.
  - The Courses shall be completed within the first III Semesters of the Programme.
  - The allotment of credits is as follows
    - 4 weeks Course - 1 credit
    - 8 weeks Course - 2 credits
    - 12 weeks Course - 3 credits

### ELIGIBILITY FOR THE DEGREE

- The candidate will not be eligible for the Degree without completing the prescribed Courses of study and a minimum of 50% Pass marks in all the Courses.
  - No Pass minimum for Internal Assessment for other Courses.
  - Pass minimum for External Examination is 27 marks out of 60 marks for Core Courses, Discipline Specific Elective Courses and Non Major Elective Course.
  - Pass minimum for Practice for SET/NET - General Paper is 50 Marks.
- **Attendance**
  - The students who have attended the classes for 76 days (85%) and above are permitted to appear for the Summative Examinations without any condition.
  - The students who have only 60-75 days (66% - 84%) of attendance are permitted to appear for the Summative Examinations after paying the required fine amount and fulfilling other conditions according to the respective cases.
  - The students who have attended the classes for 59 days and less – upto 45 days (50% - 65%) can appear for the Summative Examinations only after getting special permission from the Principal.

- The students who have attended the classes for 44 days or less (<50%) cannot appear for the Summative Examinations and have to repeat the whole semester.
  - These rules are applicable to UG, PG and M.Phil. Programmes and come into effect from 2020-2021 onwards.
  - For Certificate, Diploma, Advanced Diploma and Post Graduate Diploma Programmes, the students require 75% of attendance to appear for the Theory/Practical Examinations.

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### **B.3 ASSESSMENT MANAGEMENT PLAN**

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An Assessment Management Plan that details the assessment strategy both at the Programme and the Course levels is prepared. The continuous assessment is implemented using an assessment rubric to interpret and grade students.

#### **B.3.1 Assessment Process for CO Attainment**

Assessment is one or more processes carried out by the institution that identify, collect and prepare data to evaluate the achievement of Course Outcomes and Programme Outcomes. Course Outcome is evaluated based on the performance of students in the Continuous Internal Assessments and in End Semester Examination of a course. Target levels of attainment shall be fixed by the Course teacher and Heads of the respective departments.

**Direct Assessment (Rubric based)** - Conventional assessment tools such as Term Test, Assignment, Quiz and End Semester Summative Examination are used.

**Indirect Assessment** - Done through Course Exit Survey.

#### **CO Assessment Rubrics**

For the evaluation and assessment of COs and POs, rubrics are used. Internal assessment contributes 40% and End Semester assessment contributes 60% to the total attainment of a CO for the theory courses. For the practical courses, internal assessment contributes 50% and Semester assessment contributes 50% to the total attainment of a CO. Once the Course Outcome is measured, the PO can be measured using a CO-PO matrix.

## CO Attainment

### Direct CO Attainment

Course Outcomes of all courses are assessed and the CO - wise marks obtained by all the students are recorded for all the assessment tools. The respective CO attainment level is evaluated based on set attainment rubrics.

### Attainment Levels of COs

Assessment Methods	Attainment Levels	
Internal Assessment	Level 1	50% of students scoring more than average marks or set target marks in Internal Assessment tools
	Level 2	55% of students scoring more than average marks or set target marks in Internal Assessment tools
	Level 3	60% of students scoring more than average marks or set target marks in internal Assessment tools
End Semester Summative Examination	Level 1	50% of students scoring more than average marks or set target marks in End Semester Summative Examination
	Level 2	55% of students scoring more than average marks or set target marks in End Semester Summative
	Level 3	60% of students scoring more than average marks or set target marks in End Semester Summative Examination

### Target Setting for Assessment Method

For setting up the target of internal assessment tools, 55% of the maximum mark is fixed as target. For setting up the target of End Semester Examination, the average mark of the class shall be set as target.

### Formula for Attainment for each CO

Attainment = Percentage of students who have scored more than the target marks

$$\text{Percentage of Attainment} = \frac{\text{Number of Students who Scored more than the Target}}{\text{Total Number of Students}} \times 100$$

### Indirect CO Attainment

At the end of each Course, an exit survey is conducted to collect the opinion of the students on attainment of Course Outcomes. A questionnaire is designed to reflect the views of the students about the attainment of Course Outcomes.

### Overall CO Attainment=75% of Direct CO Attainment + 25 % of Indirect CO Attainment

In each Course, the level of attainment of each CO is compared with the predefined targets. If the target is not reached, the Course teacher takes necessary steps for the improvement to reach the target.

For continuous improvement, if the target is reached, the Course teacher can set the target as a value greater than the CO attainment of the previous year.

### B.3.2 Assessment Process for Overall PO Attainment

With the help of CO against PO mapping, the PO attainment is calculated. PO assessment is done by giving 75% weightage to direct assessment and 25% weightage to indirect assessment. Direct assessment is based on CO attainment, where 75% weightage is given to attainment through End Semester examination and 25 % weightage is given to attainment through internal assessments. Indirect assessment is done through Graduate Exit Survey and participation of students in Co-curricular/Extra curricular activities.

### PO Assessment Tools

Mode of Assessment	Assessment Tool	Description
Direct Attainment (Weightage -75%)	CO Assessment	This is computed from the calculated CO Attainment value for each Course
Indirect Attainment (Weightage - 25%)	Graduate Exit Survey 10%	At the end of the Programme, Graduate Exit Survey is collected from the graduates and it gives the opinion of the graduates on attainment of Programme Outcomes
	Co-curricular / Extra curricular activities 15%	For participation in Co-curricular/Extra curricular activities during the period of their study.

**Programme Articulation Matrix (PAM)**

Course Code	Course Title	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8
Average Direct PO Attainment									
Direct PO Attainment in percentage									

**Indirect Attainment of POs for all Courses**

POs	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8
Graduate Exit Survey								
Indirect PO Attainment								

**Attainments of POs for all Courses**

POs	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8
Direct Attainment(Weightage - 75%)								
Indirect Attainment(Weightage - 25%)								
Overall PO Attainment								

**Overall PO Attainment = [ 75% of Direct PO Attainment +  
25% of Indirect PO Attainment (Graduate Exit Survey  
& Participation in Co- curricular and  
Extra curricular Activities)]**

**Expected Level of Attainment for each of the Programme Outcomes**

POs	Level of Attainment
Value $\geq$ 70%	Excellent
Value $\geq$ 60 % and Value $<$ 70%	Very Good
Value $\geq$ 50 % and Value $<$ 60%	Good
Value $\geq$ 40% and Value $<$ 50%	Satisfactory
Value $<$ 40%	Not Satisfactory

**Level of PO Attainment**

<b>Graduation Batch</b>	<b>Overall PO Attainment (in percentage)</b>	<b>Whether Expected Level of PO is Achieved?</b>

**B.3.3 Assessment Process for PEOs**

The curriculum is designed so that all the courses contribute to the achievement of PEOs. The attainment of PEOs is measured after 3 years of completion of the Programme only through Indirect methods.

**Target for PEO Attainment**

<b>Assessment Criteria</b>	<b>Target (UG)</b>	<b>Target (PG)</b>
Record of Employment	25 % of the class strength	30 % of the class strength
Progression to Higher Education	40 % of the class strength	5 % of the class strength
Record of Entrepreneurship	2 % of the class strength	5 % of the class strength

**Attainment of PEOs**

<b>Assessment Criteria &amp; Tool</b>	<b>Weightage</b>
Record of Employment	10
Progression to Higher Education	20
Record of Entrepreneurship	10
Feedback from Alumnae	30
Feedback from Parents	10
Feedback from Employers	20
<b>Total Attainment</b>	<b>100</b>

$$\text{Percentage of PEO Attainment from Employment} = \frac{\text{Number of Students who have got Employment}}{\text{Target}} \times 100$$

$$\text{Percentage of PEO Attainment from Higher Education} = \frac{\text{Number of Students who pursue Higher Education}}{\text{Target}} \times 100$$

$$\text{Percentage of PEO Attainment from Entrepreneurship} = \frac{\text{Number of Students who have become Entrepreneurs}}{\text{Target}} \times 100$$

### Expected Level of Attainment for each of the Programme Educational Objectives

POs	Level of Attainment
Value $\geq$ 70%	Excellent
Value $\geq$ 60 % and Value $<$ 70%	Very Good
Value $\geq$ 50 % and Value $<$ 60%	Good
Value $\geq$ 40% and Value $<$ 50%	Satisfactory
Value $<$ 40%	Not Satisfactory

#### Level of PEO Attainment

Graduation Batch	Overall PEO Attainment (in percentage)	Whether Expected Level of PEO is Achieved?

### C. PROCESS OF REDEFINING THE PROGRAMME EDUCATIONAL OBJECTIVES

The college has always been involving the key stake holders in collecting information and suggestions with regard to curriculum development and curriculum revision. Based on the information collected, the objectives of the Programme are defined, refined and are inscribed in the form of PEOs. The level of attainment of PEOs defined earlier will be analysed and will identify the need for redefining PEOs. Based on identified changes in terms of curriculum, regulations and PEOs, the administrative system like Board of Studies, Academic Council and Governing Body may recommend appropriate actions. As per the Outcome Based Education Framework implemented from the Academic Year 2020 -2021, the following are the Programme Structure, the Programme Contents and the Course Contents of M.Sc. Chemistry Programme.



# V.V.VANNIAPERUMAL COLLEGE FOR WOMEN

Curriculum for M.Sc. Chemistry

(Belonging to Virudhunagar Hindu Nadars)

An Autonomous Institution Affiliated to Madurai Kamaraj University, Madurai

Re-accredited with 'A' Grade (3<sup>rd</sup> Cycle) by NAAC

VIRUDHUNAGAR - 626 001

## MASTER OF SCIENCE- CHEMISTRY (7019)

*Outcome Based Education with Choice Base Credit System*

Programme Structure - Allotment of Hours and Credits

For those who join in the Academic Year 2020-21

Components	Semester				Total Number of Hours (Credits)
	I	II	III	IV	
Core Course	6 (4)	6 (4)	6 (4)	6 (5)	24 (17)
Core Course	6 (5)	6 (5)	6 (5)	6 (5)	24 (20)
Core Course	6 (5)	6 (5)	6 (5)	6 (5)	24 (20)
Core Course Practical	6 (3)	6 (3)	6 (3)	6(4)	24 (13)
Project	-	-	-	6 (5)	6(5)
Discipline Specific Elective Course	6 (5)	6 (5)	-	-	12 (10)
Non Major Elective Course	-	-	5 (4)	-	5 (4)
Online Course	-	-	1 (1)	-	1 (1)
<b>Total</b>	<b>30 (22)</b>	<b>30 (22)</b>	<b>30 (22)</b>	<b>30 (24)</b>	<b>120 (90)</b>
Extra Credit Course(Optional) - MOOC	-	-	-	-	Limited to a maximum of 15 credits



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## M.Sc. CHEMISTRY SEMESTER-I PROGRAMME CONTENT

S.No.	Components	Title of the Course	Course Code	Hours per Week	Credits	Exam. Hours	Marks		
							Int.	Ext.	Total
1	Core Course-1	Introduction to Organic Reactions	20PCHC11	6	4	3	40	60	100
2	Core Course-2	Chemical Bonding, Solid state and Bioinorganic Chemistry	20PCHC12	6	5	3	40	60	100
3	Core Course-3	Quantum Mechanics and Thermodynamics	20PCHC13	6	5	3	40	60	100
4	Core Practical-1	Organic Qualitative and Quantitative Analyses	20PCHC11P	6	3	6	40	60	100
5	DSEC-1	Medicinal and Pharmaceutical Chemistry / Computers in Chemistry/Dye Chemistry	20PCHE11/ 20PCHE12/ 20PCHE13	6	5	3	40	60	100
<b>Total</b>				<b>30</b>	<b>22</b>				<b>500</b>

DSEC: Discipline Specific Elective Course

**SEMESTER II**

S.No.	Components	Title of the Course	Course Code	Hours per Week	Credits	Exam. Hours	Marks		
							Int.	Ext.	Total
1	Core Course-4	Stereochemistry and Reaction Mechanism	20PCHC21	6	4	3	40	60	100
2	Core Course-5	Coordination Chemistry and f-block elements	20PCHC22	6	5	3	40	60	100
3	Core Course-6	Group theory, Statistical Thermodynamics and Macromolecular Chemistry	20PCHC23	6	5	3	40	60	100
4	Core Practical-2	Inorganic Qualitative Analysis and Complexometric Titration with EDTA	20PCHC21P	6	3	6	40	60	100
5	DSEC-2	Analytical Chemistry / Polymer Chemistry / Environmental Chemistry	20PCHE21/ 20PCHE22/ 20PCHE23	6	5	3	40	60	100
<b>Total</b>				<b>30</b>	<b>22</b>				<b>500</b>

DSEC: Discipline Specific Elective Course

**SEMESTER III**

S.No.	Components	Title of the Course	Course Code	Hours per Week	Credit	Exam Hours	Marks		
							Int.	Ext.	Total
1	Core Course-7	Organic Spectroscopy, Rearrangement, Reagents and Synthetic Methods	20PCHC31	6	4	3	40	60	100
2	Core Course-8	Organometallics, Nuclear Chemistry and Inorganic spectroscopy	20PCHC32	6	5	3	40	60	100
3	Core Course-9	Electrochemistry and Molecular Spectroscopy	20PCHC33	6	5	3	40	60	100
4	Core Practical-3	Physical Chemistry Experiments	20PCHC31P	6	3	6	40	60	100
5	NMEC	NME – Chemistry for Competitive Examination	20PCHN31	5	4	3	40	60	100
6	Online Course	Practice for CSIR NET – General Paper	20PGOL32	1	1	-	100	-	100
<b>Total</b>				<b>30</b>	<b>22</b>				<b>600</b>

NMEC: Non Major Elective Course

## SEMESTER IV

S.No	Components	Title of the Course	Course Code	Hours per Week	Credits	Exam. Hours	Marks		
							Int	Ext	Total
1	Core Course-10	Heterocycles , Natural Products and Analytical Techniques	20PCHC41	6	5	3	40	60	100
2	Core Course-11	Chemical Kinetics, Surface and Biophysical Chemistry	20PCHC42	6	5	3	40	60	100
3	Core Course-12	Nano and Green Chemistry	20PCHC43	6	5	3	40	60	100
3	Core Practical-4	Inorganic Quantitative Analysis and Complex Preparation	20PCHC41P	6	4	6	40	60	100
4	Core Project	Project Viva - Voce	20PCHC41PR	6	5	6	40	60	100
<b>Total</b>				<b>30</b>	<b>24</b>		<b>500</b>		



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VIRUDHUNAGAR - 626 001

### REVISED PROGRAMME CONTENT

#### M.Sc. CHEMISTRY

#### SEMESTER-I

S.No.	Components	Title of the Course	Course Code	Hours per Week	Credits	Exam. Hours	Marks		
							Int.	Ext.	Total
1	Core Course-1	Introduction to Organic Reactions	20PCHC11	6	4	3	40	60	100
2	Core Course-2	Chemical Bonding, Solid state and Bioinorganic Chemistry	20PCHC12	6	5	3	40	60	100
3	Core Course-3	Quantum Mechanics and Thermodynamics	20PCHC13	6	5	3	40	60	100
4	Core Practical-1	Organic Qualitative and Quantitative Analyses	20PCHC11P	6	3	6	40	60	100
5	DSEC-1	Medicinal and Pharmaceutical Chemistry / Computers in Chemistry/Dye Chemistry	20PCHE11/ 20PCHE12/ 20PCHE13	6	5	3	40	60	100
<b>Total</b>				<b>30</b>	<b>22</b>				<b>500</b>

DSEC: Discipline Specific Elective Course

**SEMESTER II**

S.No.	Components	Title of the Course	Course Code	Hours per Week	Credits	Exam. Hours	Marks		
							Int.	Ext.	Total
1	Core Course-4	Stereochemistry and Reaction Mechanism	20PCHC21N	6	4	3	40	60	100
2	Core Course-5	Coordination Chemistry and f-block elements	20PCHC22N	6	5	3	40	60	100
3	Core Course-6	Group theory, Statistical and Non-Equilibrium Thermodynamics	20PCHC23N	6	5	3	40	60	100
4	Core Practical-2	Inorganic Qualitative Analysis and Complexometric Titration with EDTA	20PCHC21P	6	3	6	40	60	100
5	DSEC-2	Analytical Chemistry / Polymer Chemistry / Industrial Chemistry	20PCHE21N/ 20PCHE22/ 20PCHE23	6	5	3	40	60	100
<b>Total</b>				<b>30</b>	<b>22</b>				<b>500</b>

DSEC: Discipline Specific Elective Course

**SEMESTER III**

S.No.	Components	Title of the Course	Course Code	Hours per Week	Credit	Exam Hours	Marks		
							Int.	Ext.	Total
1	Core Course-7	Organic Spectroscopy, Rearrangement, Reagents and Synthetic Methods	20PCHC31N	6	4	3	40	60	100
2	Core Course-8	Organometallics, Inorganic photochemistry and spectroscopy	20PCHC32N	6	5	3	40	60	100
3	Core Course-9	Electrochemistry and Molecular Spectroscopy	20PCHC33N	6	5	3	40	60	100
4	Core Practical-3	Physical Chemistry Experiments	20PCHC31P	6	3	6	40	60	100
5	NMEC	NME – Chemistry for Competitive Examination	20PCHN31N	5	4	3	40	60	100
6	Online Course	Practice for CSIR NET – General Paper	20PGOL32	1	1	-	100	-	100
<b>Total</b>				<b>30</b>	<b>22</b>				<b>600</b>

NMEC: Non Major Elective Course

Curriculum for M.Sc., Chemistry  
**SEMESTER IV**

S.No	Components	Title of the Course	Course Code	Hours per Week	Credits	Exam. Hours	Marks		
							Int	Ext	Total
1	Core Course-10	Heterocycles , Natural Products and Analytical Techniques	20PCHC41N	6	5	3	40	60	100
2	Core Course-11	Chemical Kinetics and Catalysis, Photo, Biophysical and Supramolecular Chemistry	20PCHC42N	6	5	3	40	60	100
3	Core Course-12	Nano and Green Chemistry	20PCHC43N	6	5	3	40	60	100
4	Core Practical-4	Inorganic Quantitative Analysis and Complex Preparation	20PCHC41P	6	4	6	40	60	100
5	Core Project	Project - Research Methodology & Ethics	22PCHC41PR	6	5	6	60	40	100
<b>Total</b>				<b>30</b>	<b>24</b>				<b>500</b>



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### M.Sc. CHEMISTRY

(For those who join in the Academic Year 2020-2021)

Semester I	<b>INTRODUCTION TO ORGANIC REACTIONS</b>	Hours/Week: 6	
Core Course-1		Credits: 4	
<b>Course Code</b> <b>20PCHC11</b>		Internal 40	External 60

### COURSE OUTCOMES

On completion of the course, students will be able to

- CO1: explain electron displacement effects in covalent molecules, energy profile diagram, configuration, aromatic character and basic concepts of UV, IR and mass spectroscopy. [K2]
- CO2: interpret the methods of determination of reaction mechanism, the effect of structure and configuration on reactivity of organic compounds and their spectral values and the chemistry of novel ring systems. [K3]
- CO3: scrutinize the addition compounds, kinetic and thermodynamic requirements for reaction, erythro and threo isomers, aromatic sextet in different ring systems and the pattern of fragmentation in mass spectrum [K4]
- CO4: analyze the significance of Hammett equation, stability of reaction intermediates, relationship between symmetry and chirality of stereoisomers, distinction between alternant and non alternant hydrocarbons and the applications of UV and IR spectroscopy. [K4]
- CO5: categorize the polarization effects, mechanistic information obtained from kinetic and non-kinetic studies, stereoisomers, aromatic and non-aromatic behavior of organic compounds and the results of UV, IR and mass spectrum. [K5]

## **UNIT I**

### **Electron Displacement**

Inductive and field effects – bond distance – bond energies – delocalized bonds – cross - conjugation – rules of resonance – resonance energy – resonance effect – steric inhibition of resonance – Hyperconjugation – hydrogen bonding - addition compounds: EDA complexes – Crown ether complexes – inclusion compounds – Quantitative treatment of the effect of structure on reactivity – The Hammett relationship – significance of reaction and substituent constants – application of the Hammett equation in reaction mechanism – limitations and deviations. (18 Hours)

## **UNIT II**

### **Introduction to Reaction Mechanism**

Reaction intermediates – free radicals, carbenes, nitrenes, carbanions, carbocations – formation and stability of reaction intermediates – methods of determination of reaction mechanism: kinetic and thermodynamic control of chemical reactions. Kinetic and non-kinetic methods of determining organic reaction mechanism – Principles of microscopic reversibility – Energy profile diagram – Hammond postulate. (18 Hours)

## **UNIT III**

### **Stereochemistry – I**

Symmetry elements and point group classification – Concept of chirality - necessary and sufficient conditions for chirality – Relationship between substrate symmetry and chirality. Projection formulae –Wedge, Fischer, Sawhorse and Newmann. Optical isomerism due to centre of chirality. Molecules with one stereogeniccentre (chiral centre) and molecules with more than one chiral centre. Properties of enantiomers and diastereoisomers. Erythro and threo nomenclature. Configuration – determination of configuration. Cahn Ingold and Prelog system of designation of configuration.

### **Geometrical Isomerism:**

E-Z nomenclature – determination of configuration of geometrical isomers using physical and chemical methods – stereoisomerism in monocyclic compounds (upto six membered ring) (18 Hours)

## **UNIT IV**

### **Aromatic Character**

Aromatic character in benzene, five, seven and eight membered rings – other systems with aromatic sextets – Huckel's rule – Craig's rule – concept of alternant and non-alternant hydrocarbons, homoaromaticity and anti-aromaticity. Chemistry of cyclopentadienyl anion – Fulvene, Azulene, Tropolones, Sydnones and Annulenes.

**Novel ring systems:**

Nomenclature of bi-cyclic and tri-cyclic systems – chemistry of adamantane, cubane and catenanes. (18 Hours)

**UNIT V****Spectroscopy**

UV Spectroscopy : Principle - absorption spectra of conjugated dienes -  $\alpha$ ,  $\beta$ -unsaturated carbonyl compounds - Woodward - Fieser rules.

IR Spectroscopy : Molecular vibrations - vibrational frequency - factors influencing group frequencies - quantitative studies.

Applications of UV and IR spectroscopy in distinguishing axial and equatorial conformers, inter-and intra-molecular hydrogen bonding and keto-enol tautomerism.

Mass spectrometry : Principle - type of ions-base peak - parent ion, metastable and isotopic peaks - fragmentation - general rules - pattern of fragmentation for various classes of compounds - McLafferty rearrangement - Retro Diels - Alder reaction. (18 Hours)

**TEXT BOOKS**

1. Ahluwalia, V.K. (2015). *Organic Reaction Mechanism*. New Delhi: Narosa Publishing House, 4<sup>th</sup> Edition.
2. Chatwal, G.R. (2014). *Reaction Mechanism and Reagents in Organic Chemistry*. Mumbai: Himalaya Publishing House, 5<sup>th</sup> Edition.
3. Ramesh, P. (2005). *Basic Principles of Organic Stereochemistry*. Madurai: Meenu Publishers, 1<sup>st</sup> Edition.
4. Sharma, Y.R. (2018). *Elementary Organic Spectroscopy*. New Delhi: S Chand Company(P) Ltd, 5<sup>th</sup> Edition.

**REFERENCE BOOKS**

1. Sykes, P. (2013). *Guidebook to Mechanism in Organic Chemistry*. Singapore: Pearson Education Ltd, 6<sup>th</sup> Edition.
2. Jerry March. (2010). *Advanced Organic Chemistry*. New Jersey: John Wiley & Sons. 4<sup>th</sup> Edition.
3. Gould, E.S. (1959). *Mechanism and Structure in Organic Chemistry*. New York: Henry Holt & Co, 1<sup>st</sup> Edition.
4. Finar, I.L. (2003). *Organic Chemistry*. Vol.I, Singapore: Pearson Education 5<sup>th</sup> Edition.

5. Nasipuri, D. (2004). *Stereochemistry of Organic Compounds*. New Delhi: New Age International (P) Ltd.
6. Kalsi, P.S. (2015). *Stereochemistry, Conformation and Mechanism*. New Delhi: New Age International Publishers, 8<sup>th</sup> Edition.
7. Dyer, R. (2010). *Application of Absorption Spectroscopy of Organic Compounds*. New Delhi: PHI Learning Pvt. Ltd, 1<sup>st</sup> Edition.
8. Kemp, (2009). *Organic Spectroscopy*. New York: Palgrave, 3<sup>rd</sup> Edition.
9. Silverstein, M. & Webster, X. (2004). *Spectrometric Identification of Organic Compounds*. New Jersey: John Wiley & Sons, 6<sup>th</sup> Edition.

Course Code 20PCHC11	PO1		PO2	PO3		PO4	PO5	PO6	PO7	PO8
	PSO 1.a	PSO 1.b	PSO 2	PSO 3.a	PSO 3.b	PSO 4	PSO 5	PSO 6	PSO 7	PSO 8
CO1	H	H	M	H	H	H	M	M	H	M
CO2	H	H	M	M	M	H	M	L	H	M
CO3	H	H	M	M	M	H	M	L	H	M
CO4	H	H	M	M	M	H	M	M	H	M
CO5	H	H	M	H	H	H	M	H	H	M

Dr. J.Kavitha  
Head of the Department

Mrs.R.Nagasathya  
Mrs. A.Prasanna  
Course Designers



**M.Sc. CHEMISTRY**  
**(For those who join in the Academic Year 2020-2021)**

Semester I	<b>CHEMICAL BONDING, SOLID STATE AND BIOINORGANIC CHEMISTRY</b>	Hours/Week: 6	
Core Course-2		Credits: 5	
Course Code <b>20PCHC12</b>		Internal 40	External 60

### COURSE OUTCOMES

On completion of the course, the students shall be able to

CO1: understand the concepts of bonding, electronic structure of atoms, solid state, bioinorganic, photo electron and Mossbauer spectroscopy. [K2]

CO2: illustrate the nature of chemical bonds, bond properties and electrostatic interactions. [K3]

CO3: predict the binding energy, stoichiometric defects of crystals and functions of metal in oxidases. [K3]

CO4: analyse the structure and bonding of molecules, conducting ability of solids, low spin and high spin complexes using Mossbauer Spectroscopy and XPES. [K4]

CO5: evaluate the importance and basic idea about the chemical bonding, solid state and bioinorganic chemistry, PES and Mossbauer Spectroscopy. [K5]

### UNIT I Nature of the chemical bond

Ionic bond – Lattice energy and its determination by Born-Haber cycle and Born-Landé Equation – electrical conductivity and solubility of ionic compounds – ionic radii. Goldschmidt's radius ratio. Calculation of ionic radius – Pauling's method and Linde's method. Effective nuclear charge-Slater's rule.

Covalent bond – qualitative treatment of valence bond theory – Heitler-London theory – Pauling theory -Bond properties, bond order, bond energy, bond length and bond polarity. Partial ionic character of covalent bonds-Fajan's Rule –Effects of polarization-Drawbacks of VSEPR Theory –Walsh Diagrams- Bent's rule - VSEPR theory and its applications to  $ICl_2^-$ ,  $IF_5$ ,  $IF_7$ ,  $ClO_4^-$  ions. VSEPR applied to Xenon halides. (18 Hours)

**UNIT II Bonding application and Chemistry of non-aqueous solvents**

Molecular orbital theory LCAO theory – Hybridisation and resonance. Application of VB and MO theories to the structure of heteronuclear diatomic(NO, HCl, HF) and selective polyatomic molecules ( $\text{CO}_3^{2-}$ ,  $\text{NO}_2$ ,  $\text{BeH}_2$ ,  $\text{CO}_2$ ) comparison of VB and MO theories.

A general study of the typical reactions in dinitrogen tetroxide, anhydrous hydrogen fluoride, sulphuric acid - HSAB concept of acids and bases -acid, base strength and hardness and softness -symbiosis - theories of hardness and softness (18 Hours)

**UNIT III Solid State Chemistry**

Packing of atoms and ions- close packing arrangements-HCP, CCP and BCC lattice. Radius ratio rules- Limiting radius ratio. Structure of typical lattices such as calcite, cesium chloride, Nickel arsenide, Fluorite, Antifluorite, Cadmium iodide, Perovskite, Spinel (normal and inverse). Bragg's equation- problems involving Bragg's equation. Crystal structure determination- X-ray diffraction study, Electron and Neutron diffractions Crystal defects- point – Schotky and Frenkel defect - line and plane defects- Non-Stoichiometric Defects- colour centers- Solid electrolytes and their application- Band Theory- bonding in metals – Free electron theory- Optical and electrical properties of semiconductors. Superconductivity: High temperature super conductors, properties and applications-BCS Theory- Cooper electrons- Meissener effect and Levitation. (18 Hours)

**UNIT IV Bio-inorganic Chemistry**

Essential and trace elements in biological systems –metalloporphyrins – the porphyrine ring system – chlorophyll – photosynthetic electron transfer - Electron transport sequence – biological electron transfer – electron transfer agents – cytochromes – Hemoglobin – myoglobins – and synthetic oxygen carriers – nitrogen fixation – in vivo and in vitro – copper proteins-Metal complexes in medicine- Biomineralisation of iron-Metal complexes in medicine-Chelate therapy- Metals used for diagnosis and chemotherapy- metal-nucleic acid interactions. (18 Hours)

**UNIT V****a) Photo Electron Spectroscopy (PES)**

Theory – XPS - UV- PES- Instrumentation evaluation of ionization potential – chemical identification of elements - Koopmann's theorem – chemical shift – UPS – XPES of

N<sub>2</sub>, O<sub>2</sub>, NH<sub>3</sub>, H<sub>2</sub>O and CH<sub>4</sub> – evaluation of vibrational constants from UPS – spin orbit coupling – Auger spectroscopy – principle and its applications. (18 Hours)

#### b) Mossbauer spectroscopy

Mossbauer effect resonance absorption – Doppler effect – Doppler velocity – Experimental technique of measuring resonance absorption – isomer shift- effect of quadrupole nucleus – magnetic hyperfine splittings – applications of Mossbauer spectroscopy in the study of iron and tin complexes. (18 Hours)

#### TEXT BOOKS

1. Sathya Prakash, Tuli, G.D. Basu, S.K. Madan, R.D. (2011). *Advanced inorganic chemistry*. Volume I, New Delhi: S.Chand & Company Ltd., 19<sup>th</sup> Edition.
2. Azaroff, V. (1989). *Introduction to Solids*. New York: Tata Ma Graw-Hill Publishing Company Ltd., 1<sup>st</sup> Edition.
3. Das, A.K. (2016). *Bioinorganic Chemistry*. New Delhi: Arunabha Sen Books and Allied (P) Ltd., 1<sup>st</sup> Edition.
4. Madan, R.D. (2018). *Modern Inorganic Chemistry*. New Delhi: S.Chand and Company Pvt.Ltd., 3<sup>rd</sup> Edition.

#### REFERENCE BOOKS

1. Huheey, E. Keitler, A. and Keitler, L. (2006), *Inorganic Chemistry*. New York: Harper, Dorling Kindersley Pvt. Ltd., 4<sup>th</sup> Edition.
2. Hussain Reddy, K. (2017). *Bioinorganic Chemistry*. New Delhi: New Age International (P) Ltd., Publishers. 1<sup>st</sup> Edition.
3. Cotton, F.A & Wilkinson, G. (2007). *Advanced Inorganic Chemistry*. Singapore: John, Wiley & sons, PTE Ltd., 6<sup>th</sup> Edition.
4. Purcell, K. F & Kotz. (2010). *Inorganic Chemistry*. US: Cengage Learning India Pvt.Ltd., Boston. 1<sup>st</sup> Edition.
5. Sharpe, A.G. (2007). *Inorganic Chemistry*. London: Pearson Education Ltd. 3<sup>rd</sup> Edition.

Course Code 20PCHC12	PO1		PO2	PO3		PO4	PO5	PO6	PO7	PO8
	PSO 1.a	PSO 1.b	PSO 2	PSO 3.a	PSO 3.b	PSO 4	PSO 5	PSO 6	PSO 7	PSO 8
CO1	H	H	M	H	H	H	H	H	H	H
CO2	H	H	H	H	H	H	M	M	H	H
CO3	H	H	M	M	H	H	H	M	H	M
CO4	H	H	M	M	H	H	M	M	M	M
CO5	H	H	M	H	M	M	H	M	H	M

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Dr. M. Vairalakshmi  
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### M.Sc. CHEMISTRY

(For those who join in the Academic Year 2020-2021)

Semester I	<b>QUANTUM MECHANICS AND THERMODYNAMICS</b>	Hours/Week: 6	
Core Course-3		Credits: 5	
Course Code <b>20PCHC13</b>		Internal 40	External 60

#### COURSE OUTCOMES

On completion of the course, the students shall be able to

CO1: explain the theory and concepts of Quantum mechanics and thermodynamics.

[K2]

CO2: apply the knowledge of quantum mechanics to simple systems and illustrate the concepts of thermodynamics. [K3]

CO3: interpret advance knowledge on chemical thermodynamics and quantum mechanics and employ the chemistry of phase rule. [K3]

CO4: calculate approximation methods in Quantum mechanics and derive thermodynamic relations. [K4]

CO5: assess the relation between the thermodynamic and electrochemical parameters and evaluate the theorems in quantum mechanics. [K5]

#### UNIT I The Birth Of Quantum Mechanics

Deviations from classical mechanics - Planck's concept of black-body radiation – de-Broglie's concept of matter waves – Heisenberg's uncertainty principle and complementarity. Operators – Linear operators – commutation relations – Method of getting the following quantum mechanical operators – Position, Momentum, Kinetic energy, Potential energy, Total energy and Angular momentum – Ladder operator.

Postulates of quantum mechanics – Hermiticity and proving that quantum mechanical operators are Hermitian – Eigen value and Eigen function – Orthogonality and Normalization of wave functions. (18 Hours)

**UNIT III Application of Quantum Mechanics to Simple Systems**

Derivation of Schrodinger wave equation – Application to SWE to simple systems – Free particle – Particle moving in one dimensional box – Particle moving in 3D box - Particle moving in a Ring – Rigid rotator – Spherical harmonics – Simple Harmonic Oscillator – Hermite Polynomials – Hydrogen atom problem – radial wave function – Radial Probability Distribution – Shapes of various atomic orbitals. (18 Hours)

**UNIT III Approximation methods in Quantum Mechanics:**

Need for approximation methods – Schrodinger equation for Helium atom and many electron systems – The Time independent Perturbation theory (first order only) – Application to Hydrogen atom – Variation theorem – Application to Hydrogen and Helium atom – Hartee-Fock-Self Consistent(HFSCF) method of many electron system – Application to Helium atom – Electron spin and Pauli principle – Antisymmetric nature of wave functions – Slater determinants – Born-Oppenheimer approximation – Born-Oppenheimer break-down – VB and MO theories. (18 Hours)

**UNIT IV Thermodynamics – I**

Brief resume of concepts of First law and Second law of Thermodynamics – Gibbs and Helmholtz free energy – Entropy – Entropy as criteria for spontaneity – Entropy of mixing – Partial molar properties – Determination of partial molar properties – Gibbs-Duhem equation – Gibbs-Duhem-Marculus equation – Maxwell's relations – Equilibrium constants – Dependence of temperature on equilibrium constants – Concepts of Fugacity – Determination of fugacity - Third law of Thermodynamics – Absolute entropies – Determination of Absolute entropies – Exception to Third law - -Unattainability of absolute zero. (18 Hours)

**UNIT V Thermodynamics – II**

Van't Hoff isochore – van't Hoff isotherm – Standard reaction free energy – its calculation from thermochemical, electrochemical and equilibrium data – Temperature coefficient of reaction free energy and equilibrium constant – Thermodynamic explanation of the Le Chatelier principle – Gibbs phase rule – its thermodynamic derivation – Application of phase rule to three component systems – Formation of one-pair, two-pairs and three-pairs of partially miscible liquids – Systems composed of two solids and a liquid. (18 Hours)

**TEXT BOOKS**

1. Chandra, A.K. (2010). *Introductory Quantum Chemistry*, New Delhi: Tata McGraw Hill Publishing Co., 4<sup>th</sup> Edition.

- Prasad, R.K. (2000). *Quantum Chemistry*, New Delhi: New Age International publishers, 4<sup>th</sup> Edition.
- House. E. (2008). *Fundamentals of Quantum Chemistry*, California: Academic Press, 2<sup>nd</sup> Edition.
- Puri, B.R. Sharma, L.R. & Pathania, M.S. (2003). *Principles of Physical Chemistry*, New Delhi: Vishal Publishing Co., Millennium Edition.
- Gurdeep Raj (2003), *Advanced physical Chemistry*, Goel Publishing Co., 25<sup>th</sup> Edition.
- Rajaram, J. & Kuriakose, J.C. (2003). *Thermodynamics*, Shoban Lal Nagin, New Delhi: Chand & Co., Ltd., 3<sup>rd</sup> Edition.
- Glasstone, S. *Thermodynamics for Chemists*, New Delhi: East-West Press (P) Ltd.,

### REFERENCE BOOKS

- McQuarrie, D.A. (2003). *Quantum Chemistry*. New Delhi: Viva Books (P) Ltd., 1<sup>st</sup> Edition.
- Atkins, P.W. (2002). *Physical Chemistry*. New York: ELPS and Oxford University press, 6<sup>th</sup> Edition.
- Levine, N. (2002). *Quantum Chemistry*. New Jersey: Prentice Hall of India (P) Ltd., 5<sup>th</sup> Edition.
- Bajpai, D.N. (2011). *Advanced Physical Chemistry*. New Delhi: S. Chand & Co., Ltd.,

Course Code 20PCHC13	PO1		PO2	PO3		PO4	PO5	PO6	PO7	PO8
	PSO 1.a	PSO 1.b	PSO 2	PSO 3.a	PSO 3b	PSO 4	PSO 5	PSO 6	PSO 7	PSO 8
CO1	H	H	M	M	H	H	H	M	M	L
CO2	H	H	H	M	H	H	H	M	M	L
CO3	H	H	H	M	H	H	H	M	M	L
CO4	H	H	H	M	H	H	H	M	M	L
CO5	H	H	H	M	H	H	H	M	M	L

Dr.J.Kavitha  
Head of the Department

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Dr.A.Anitha  
Course Designers



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## M.Sc. CHEMISTRY

(For those who join in the Academic Year 2020-2021)

Semester I	<b>Organic Qualitative and Quantitative Analyses</b>	Hours/Week: 6	
Core Practical-1		Credits: 3	
<b>Course Code 20PCHC11P</b>		Internal 40	External 60

### COURSE OUTCOMES

On completion of the course, the students shall be able to

- CO1: Separate the organic mixture by chemical methods. Detect the elements (other than C, H, and O) present in a given organic compound. [K3]
- CO2: Identify the functional groups in a given organic compound. Prepare the derivatives for the given organic compound. [K3]
- CO3: Estimate the amount of glucose by adopting different procedures and estimate amino acid viz., Glycine. [K3]
- CO4: Examine the amount of Ketonic compound and compare the amount present with the standard solution. [K4]
- CO5: Categorize the given mixtures by using chromatographic techniques. [K4]

#### 1. Qualitative analysis

Separation and analysis of two component mixtures. Identification of the components and preparation of solid derivative.

#### 2. Quantitative analysis

- a) Estimation of glucose by Lane and Eynon method and Bertrand method
- b) Estimation of glycine
- c) Estimation of formalin
- d) Estimation of methyl ketone

#### 3. Separation of mixtures by chromatographic techniques-TLC and Column

(classwork only)

Course Code 20PCHC11P	PO1		PO2	PO3		PO4	PO5	PO6	PO7	PO8
	PSO 1.a	PSO 1.b	PSO 2	PSO 3.a	PSO 3.b	PSO 4	PSO 5	PSO 6	PSO 7	PSO 8
CO1	H	H	M	H	M	H	H	M	M	H
CO2	H	H	H	H	M	H	H	M	M	H
CO3	H	H	H	H	M	H	H	M	M	H
CO4	H	H	H	H	M	H	H	M	M	H
CO5	H	H	H	H	M	H	H	M	M	H

Dr. J. Kavitha  
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Mrs. S.Lalithambigai  
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Course Designers



## V.V.VANNIAPERUMAL COLLEGE FOR WOMEN

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VIRUDHUNAGAR - 626 001

### M.Sc. CHEMISTRY

(For those who join in the Academic Year 2020-2021)

Semester I	<b>MEDICINAL AND PHARMACEUTICAL CHEMISTRY</b>	Hours/Week: 6	
DSEC – 1		Credits: 5	
Course Code <b>20PCHE11</b>		Internal 40	External 60

### COURSE OUTCOMES

On completion of the course, the students shall be able to

- CO1: understand the basic knowledge on Pharmaceutical chemistry. [K2]
- CO2: predict the structural features, synthesis and therapeutic action of antibiotics, thyroid hormones, antimalarial, antitubercular drugs. [K3]
- CO3: predict the structural features, synthesis and therapeutic action of antitubercular, antineoplastic, anti-inflammatory, antihypertensive and CNS drugs. [K3]
- CO4: interpret basic knowledge on bioinformatics in computer aided drug design analyse the synthesis and therapeutic action of chemotherapeutic agents. [K4]
- CO5: evaluate the concept of Quantitative Structure Activity Relationship and Molecular docking. [K5]

### UNIT I Fundamentals of Medicinal Chemistry

Definitions of Medicinal Chemistry, Pharmacology and molecular pharmacology- Nature and sources of drugs, routes of administration of drugs – General principle of drug action – drug action at active sites- biotransformations of drug – factors affecting the drug action – catalytic role of enzymes - major process involved in drug action- pharmacokinetics phase- Quantitative Structure Activity Relationship (QSAR) - Hansch approach- concept of bioisomerism- pharmacodynamics phase- receptors and classification of membrane bound receptors- enzyme inhibitors as drugs (illustrated with one example). (18 Hours)

### UNIT II Medicinally useful antibiotics

Structural features and mode of the following antibiotics: penicillin G, cephalosporin and their semi synthetic analogs ( $\beta$ -lactum), streptomycin (aminoglycoside), terramycin (tetracycline), erythromycin (macrolide) and chloramphenicol.

Prodrugs, classification, design, bioprecursor and application. Structural features and mode of action of  $\beta$ -lactam antibiotics. Agonist, design of agonist and its requirements- antagonist, design of antagonist – partial agonist. Biosynthesis of insulin and thyroid hormones.

(18 Hours)

### UNIT III Synthesis and Therapeutic action of certain drugs

**Antineoplastic agents:** Classification, synthesis, Assay e.g., Cyclophosphamide, Ifosfamide, Chlorambucil, Busulfan, Decarbazine, Methotrexate, Azathioprine, 6-Mercaptopurine, 5-fluorouracil, Cisplatin, Carboplatin.

**Antitubercular drugs:** Classification, Synthesis, Assay, e.g., Isoniazid, Pyrazinamide, Ethambutol, Thiacetazone, para-amino salicylic acid and Ethionamide.

**Antimalarial drugs:** Classification, synthesis, assay, e.g., Chloroquin, Primaquine, Amodiaquine, Mefloquine, Proguanil, Pyrimethamine. (18 Hours)

### UNIT IV Synthesis, Therapeutic action and SAR of certain drugs

**Anti-hypertensive drugs:** Nifedipine, Captopril, Hydralazine, Sodium nitropruside, Clonidine, methyl dopa and guanethidine.

**Anti-inflammatory drugs:** Antipyretics & Non-narcotic analgesics: Aspirin, sodium salicylate, paracetamol, phenylbutazone, oxyphenylbutazone, Ibuprofen, Diclofenac sodium.

**CNS Stimulant Drugs:** Amphetamine, caffeine, Theobromine, Theophylline, Nikethamide, Methyl phenidate and peracetum.

**CNS Depressant Drugs:** Phenelazine, Imipramine, Nortriptyline, Amitriptyline, Desipramine. (18 Hours)

### UNIT V

#### a) Bioinformatics in computer-aided Drug design:

Introduction, drug discovery process- historical perspective-hit identification – structural bioinformatics in drug discovery –some basics about in silico drug designing-SAR and QSAR technique in drug design-development of linear –free energy relationships-application of Hammett equation-Hansch equation –application of QSAR in CADD

#### b) Molecular Docking:

Introduction-flexibility calculation- Simulation techniques widely used in molecular docking-M D simulation - software for structure based drug design and molecular docking-A briefing on drug bank- auto dock-steps for flexible docking in auto dock –preparing the ligand and

the macromolecule for auto dock-auto grid- auto dock file formats-choose the docking algorithm-viewing conformational clusters by RMSD (18 Hours)

### TEXT BOOKS

- 1) Ashutosh Kar. (2010). *Medicinal Chemistry*. New Delhi: New Age International Publishers, 5<sup>th</sup> Edition.
- 2) Ahluwalia, V.K. & Madhu Chopra. (2012). *Medicinal Chemistry*. New Delhi: Ane Books Pvt.Ltd., 2<sup>nd</sup> Edition.
- 3) Sriram, D & Yogeeswari, P. (2008). *Medicinal Chemistry*. New Delhi: Pearson Education, 1<sup>st</sup> Edition.
- 4) Ilango, K & Valentina, P. (2007). *Text Book of Medicinal Chemistry*. Chennai:, Keerthi Publishers, 1<sup>st</sup> Edition.
- 5) Zhumur ghosh, Bibekan & Mallick. (2008). *Bioinformatics –Principles and Applications*. New York: Oxford University Press , 1<sup>st</sup> Edition.

### REFERENCE BOOKS

1. Patrick, G.L. (2001). *An Introduction to Medicinal Chemistry*. New York: Oxford University Press, 2<sup>nd</sup> Edition.
2. Parimoo, P. (2011). *A Text Book of Medicinal Chemistry*. New Delhi: CBS Publishers & Distributors Pvt.Ltd., 1<sup>st</sup> Edition.
3. Delgado, J.N. & Remers, W.A. (1998). *Text book of Organic, Medicinal & Pharmaceutical Chemistry*. Vol I, Philadelphia: J.B. Lippincott Company, 9<sup>th</sup> Edition.

Course Code 20PCHE11	PO1		PO2	PO3		PO4	PO5	PO6	PO7	PO8
	PSO 1.a	PSO 1.b	PSO 2	PSO 3.a	PSO 3.b	PSO 4	PSO 5	PSO 6	PSO 7	PSO 8
CO1	H	M	L	H	H	M	H	M	M	M
CO2	H	M	L	H	H	M	H	M	M	M
CO3	H	M	L	H	H	M	H	M	M	H
CO4	H	M	L	H	H	M	H	H	M	H
CO5	H	M	L	H	H	M	H	H	M	H

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Mrs. R.Nagasathya  
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Course Designers



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VIRUDHUNAGAR - 626 001

### M.Sc. CHEMISTRY

(For those who join in the Academic Year 2020-2021)

Semester I	<b>COMPUTERS IN CHEMISTRY</b>	Hours/Week: 6	
DSEC – 1		Credits: 5	
Course Code <b>20PCHE12</b>		Internal 40	External 60

### COURSE OUTCOMES

On completion of the course, the students shall be able to

CO1: understand the basic concepts of visual basics. [K2]

CO2: write the different language forms. [K3]

CO3: operate internet protocols, email and to apply database in chemistry. [K3]

CO4: infer the application of C language in chemistry. [K4]

CO5: evaluate the basic concepts of communication system. [K5]

### UNIT I Basic concepts of VB

Introduction to Visual Basic—the integrated development environment—the menu bar, the tool bar, the project explorer, the tool box, the properties of window, the form designer, the form layout, the immediate window, the elements of the interface—programming an application – common properties, common methods and common events – customizing the environment.

#### Working with forms:

The appearance of form—the startup form—loading, showing the hiding forms—elementary concepts of drag and drop operations. **Basic active X controls:** Elementary concepts of the text box control, the List box and Combo Box controls. Variables— declaring variables— variable types—strings, numeric and data variables cope and life forms of variables— constants. (18 Hours)

### UNIT II The Language forms and basic active controls

**Control flow statements:** If ... Then .... Else.

**Loop Statements:** Do.....Loop, For....Next and While–Wend-nested control statement—the exit statement.

**Arrays:** Declaring arrays– specifying arrays– multidimensional arrays.

**Procedures:** Subroutines, functions, calling procedures–arguments–arguments passing mechanism– using optional arguments– functions returning arrays (18 Hours)

### **UNIT III Applications of VB&C language in Chemistry**

#### **Applications of VB**

1. Calculation of molecular weight of organic compound
2. Ionic strength of an electrolyte
3. Unit cell dimensions
4. Thermodynamic parameters
5. Half-life period of a radioactive material
6. Reduced mass
7. Empirical formula of an organic compound containing C, H, and O

#### **Applications of C**

1. Self-consistent theory of molecules – Semi empirical self-consistent field method – Hartree- Fock limit – Koopmans theorem – perturbation theory (18 Hours)

### **UNIT IV Basic concepts of communication systems**

#### **Communication systems**

Satellites – RADAR – optical fibers – advantages and disadvantages–ISDN– distributed systems– advantages and disadvantages.

**Telecommunication:** analog and digital signals– types and needs of modulations – MODEMS–telecommunication software.

**Computer networks:** an overview– communication processors–protocols–network architecture.

#### **Practicals (Classworkonly)**

1. Salient features of windows and MS Word for typing texts and equations in Chemistry– tabular columns– advanced concepts.
2. Basic concept of creating and accessing databases using MS Access.
3. Significance of Chemdraw– drawing chemical structures and pasting them in the text (18 Hours)

### **UNIT V Basic concepts of internet and applications in chemistry**

#### **Internet**

History of internet–the working way of internet–getting connected to internet– internet protocols – internet addressing– domain names – internet services.

**WWW:** Web pages – home pages– web browsers– search engines – internet chat– chatting on web.

**E-mail:** Introduction–working way–mailing basics–e-mail ethics–advantages and disadvantages – creating e-mail – receiving and sending e-mails.

**Intranet:** Characterization– advantages – drawbacks– need for intranet–extranet.

**Application of internet in chemistry:** Websites in literature surveyin Chemistry– popular websites in chemistry– databases in chemistry – URLs – WAIS – downloading the attachment / PDF files–opening, browsing and searching a website–literature searching online.

**Practical (Class work only)**

Creating e-mail id, sending and receiving e-mails, attachment files, pdf files. Opening, Browsingandsearchingawebsite–downloading–literaturesurveyinchemistry–online searching. (18 Hours)

**TEXT BOOKS**

1. Raman, K.V. (1993).*Computers in Chemistry*.NewDelhi: Tata-McGraw Hill publishing Company, 1<sup>st</sup>Edition.
2. David Jung, Pierre Boutquin, John Conley,Loren Eidahl, D.LowellMauer and JackPudum.(1999).*Visual Basic 6 super bible*.NewDelhi:Techmedia,1<sup>st</sup>Edition.
3. Riyazuddin, P. (2011).*Computers in Chemistry*. New Delhi:I.K.International Publishing House Pvt.Ltd. 1<sup>st</sup>Edition.

**REFERENCE BOOKS**

1. Evangelos Petroustos, (1998). *Mastering Visual Basic 6*. New Delhi: BPBpublication,1<sup>st</sup>Edition.
2. GaryCornel, (1998).*Visual Basic 6*. New Delhi: Tat-McGraw Hill, 1<sup>st</sup> Edition.
3. Barbara Kasser, (1998).*Using the internet*.Indiana U.S.: Que Pub Publisher, 4<sup>th</sup>Edition.  
Alexis Leon& Mathews Leon(1999).*Fundamentals of Information Technology*. Chennai:Leon Vikas, 1<sup>st</sup>Edition.

Course Code 20PCHE12	PO1		PO2	PO3		PO4	PO5	PO6	PO7	PO8
	PSO 1.a	PSO 1.b	PSO 2	PSO 3.a	PSO 3.b	PSO 4	PSO 5	PSO 6	PSO 7	PSO 8
CO1	H	M	L	M	H	M	H	H	H	M
CO2	H	M	L	M	H	M	H	H	H	M
CO3	H	M	L	M	H	M	H	H	H	M
CO4	H	M	L	M	H	M	H	H	H	M
CO5	H	M	L	M	H	M	H	H	H	M

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Head of the Department

Dr.J.Kavitha  
Dr.A.Anitha  
Course Designers



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VIRUDHUNAGAR - 626 001

### M.Sc. CHEMISTRY

(For those who join in the Academic Year 2020-2021)

Semester I	<b>DYE CHEMISTRY</b>	Hours/Week: 6	
DSEC – 1		Credits: 5	
Course Code <b>20PCHE13</b>		Internal 40	External 60

#### COURSE OUTCOMES

On completion of the course, the students shall be able to

CO1: understand the basic concepts of colour and chemical constitution of dyes. [K2]

CO2: demonstrate the mechanism of dyeing. [K3]

CO3: predict the nature and applications of vat, mordant and azo dyes. [K3]

CO4: infer the chemistry involved in the production of dyes. [K4]

CO5: evaluate the theory behind the colour and brightening of dyes. [K5]

**UNIT I: Introduction** Colour and chemical constitution - chromophore, auxochrome and resonance, various theories; History of natural and synthetic dyes; Names of commercial dyes; Study of raw materials and dyestuff intermediates; Unit operations - nitration, sulphonation, halogenation, amination, diazotisation and alkali fusion; Colour index and its significance; Classification of dyes based on chemical constitution and method of applications; General properties - linearity, coplanarity and fastness. (18 Hours)

**UNIT II: Direct, Acid and Basic Dyes** Direct cotton dyes (substantive dyes) – Classification, properties, structure and mechanism of dyeing, post treatment of dyeing; Acid dyes and Basic dyes – Classification, Characteristics, trade names, Mechanism of dyeing, Nature of affinity on cellulose and protein fibres. (18 Hours)

**UNIT III Mordant, Azo and Vat Dyes** Mordant dyes – classification, methods of application; Metal complex dyes – types of bond formation between dye and various fibres;

Azo dyes – Azoic coupling components, protective colloids, electrolytes, stabilisation of diazonium salts, principles and application; Vat dyes and solubilised vat dyes – classification, methods of application, trade names, principles and application, Stripping agents and correction of faulty dyeing. (18 Hours)

**UNIT IV Other Dyes** Chemistry involved in the production of Aniline black; Prussian black; Sulphur colours; phthalocyanines; Disperse dyes - classification based on chemical structure, properties and principles of application; Solvent soluble dyes - Nigrosines and Indulines; Cyanine dyes. (18 Hours)

**UNIT V Colour and Brightening** Fluorescent brightening agents (FBA) - Theory and applications; Identification and estimation of dyes on fibres; The action of light on dyes and dyed fibres; Mechanism of fading. (18 Hours)

**TEXT BOOKS:**

1. K. Venkataraman, (1952), *The chemistry of synthetic dyes Part I & II*, Academic Press, New York,.
2. V. A. Shenai, (1991), *Introduction to Chemistry of Dyesuffs*, Sevak Prakashan Pub., Mumbai.

**REFERENCE BOOKS:**

1. V. A. Shenai, (1987), *Chemistry of Dyes and Principles of Dyeing*, Vol.-II, Sevak Prakashan, Mumbai,.
2. V. A. Shenai, (1997), *Ecology and Textiles*, Sevak Publications, Mumbai,.
3. D. M. Nunn, (1979), *The Dyeing of Synthetic Polymer and Acetate Fibres*, Dyers Company, Publication Trust,.
4. V. A. Shenai, (1998), *Toxicity of Dyes and Intermediates*, Sevak Publications, Mumbai,.
5. Directory of safe dyes conforming to German Consumer Goods Ordinances, The Dyestuff Manufacturers Association of India, 1996.

Course Code 20PCHE13	PO1		PO2	PO3		PO4	PO5	PO6	PO7	PO8
	PSO 1.a	PSO 1.b	PSO2	PSO 3.a	PSO 3.b	PSO 4	PSO 5	PSO 6	PSO 7	PSO 8
CO1	H	M	L	M	H	M	H	L	L	M
CO2	H	M	L	M	H	M	H	L	L	M
CO3	H	M	L	M	H	M	H	L	L	M
CO4	H	M	L	M	H	M	H	L	L	M
CO5	H	M	L	M	H	M	H	L	L	M

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### M.Sc. CHEMISTRY

(For those who join in the Academic Year 2020-2021)

Semester II	<b>STEREOCHEMISTRY AND REACTION MECHANISM</b>	Hours/Week: 6	
Core Course-4		Credits: 4	
Course Code <b>20PCHC21</b>		Internal 40	External 60

### COURSE OUTCOMES

On completion of the course, students will be able to

- CO1: describe prochirality and prostereoisomerism, the conformations of acyclic and cyclic systems and the basic concepts of substitution, addition and elimination reactions. [K2]
- CO2: predict the nomenclature of prostereoisomers, interpret Cram and Prelog rules, Curtin - Hammett principle, neighbouring group participation of  $n$ ,  $\pi$  and  $\sigma$  electrons and the stereochemical factors in substitution, addition and elimination reactions. [K3]
- CO3: analyse the enantiotopic and diastereotopic ligands and faces, conformations of cyclohexanones, aldohexopyranoses and decal in and the mechanisms involved in substitution, addition and elimination reactions. [K4]
- CO4: correlate the optical isomerism in molecules with no chiral centers, conformations of acyclic and cyclic systems with their physical and chemical properties, nucleophilicity and basicity, electrophilic, nucleophilic and free radical additions and aromatic electrophilic and nucleophilic substitution reactions. [K4]
- CO5: categorize nucleophilic substitution at various carbon centers, electrophilic, nucleophilic and free radical additions to multiple bonds,  $\alpha$  - elimination,  $\beta$  - elimination and pyrolytic elimination reactions and stereospecific and stereoselective reactions. [K5]

**UNIT I Stereochemistry II**

Prochirality and prostereoisomerism, enantiotopic and diastereotopic ligands and faces and their nomenclature - pro - R and pro-S and Re and Si faces. Stereospecific and stereoselective reactions. Asymmetric synthesis : Cram and Prelog rules. Optical isomerism due to axial chirality - biphenyls, allenes and spiranes. Molecules with planar chirality - paracyclophanes, trans-cyclooctene, ansa compounds. (18 Hours)

**UNIT II Conformational analysis**

Configuration and conformation - conformations of ethane and n-butane - conformational analysis - stereoelectronic and steric factors - conformation of simple acyclic compounds - conformation of monosubstituted and disubstituted cyclohexanes - correlation of the conformation of acyclic and cyclic systems with their physical and chemical properties - conformational free energy - Curtin - Hammett principles - Quantitative treatment of mobile system - Eliel-Ro equation- conformations and reactivity of cyclohexanones - conformational analysis of aldohexopyranoses-conformation of fused ring system-decalin- conformational effects in medium sized rings –concept of I strain. (18 Hours)

**UNIT III Aliphatic nucleophilic substitution**

Nucleophilicity and basicity –  $S_N1$  and  $S_N2$  mechanisms – effect of substrate structure – effect of the attacking nucleophile – effect of the leaving group – effect of the reaction medium – ambident nucleophiles – ambident substrates – neighbouring group participation of n,  $\pi$  and  $\sigma$  electrons –  $S_Ni$  mechanism – nucleophilic substitution at an aliphatic trigonal carbon – nucleophilic substitution at allylic carbon – nucleophilic substitution at vinyl carbon.

**Aliphatic electrophilic substitution:** Electrophilic substitution at saturated carbon  $S_E1$ ,  $S_E2$  mechanisms. (18 Hours)

**UNIT IV Addition to multiple bonds**

Electrophilic, nucleophilic and free radical additions - addition to conjugated systems - orientation of the addendum - stereochemical factors in reactions like addition of hydrogen, halogens, hydrogen halides and hypohalous acids hydroboration and hydroxylation – epoxidation. Addition to carbonyl groups - mechanism of Aldol condensation - Perkin reaction - Knoevenagel reaction –Mannich reaction- Cannizzaro reaction - Benzoin condensation - Claisen ester condensation - Darzen's reaction - Reformatsky reaction - Wittig

reaction - Grignard reactions. Addition to  $\alpha$ ,  $\beta$  - Unsaturated carbonyl groups - Michael addition - Diels - Alder reaction - Esterification of acids and hydrolysis of esters.

(18 Hours)

### UNIT V Elimination Reactions and Aromatic electrophilic substitution

$\alpha$  - elimination -  $\beta$  - elimination - E1, E2 and E1cB mechanisms - stereochemistry of elimination - orientation of the double bond - effect of change in the substrate, base, leaving group and medium on E1, E2 and E1cB reactions - elimination vs substitution - pyrolytic eliminations - Bredt's rule.

Orientation - reactivity - mechanism of nitration, halogenation, Friedal - Craft's reaction and sulphonation - partial rate factors – ortho / para ratio - quantitative treatment of reactivity of the electrophile (the selectivity relationship) - Aromatic nucleophilic substitution reactions -  $S_N1Ar$ ,  $S_N2$  and benzyne mechanisms.

(18 Hours)

### TEXT BOOKS

1. Ramesh, P. (2005). *Basic Principles of Organic Stereochemistry*. Madurai: Meenu Publishers, 1<sup>st</sup> Edition.
2. Ahluwalia, V.K. (2015). *Organic Reaction Mechanism*. New Delhi: Narosa Publishing House, 4<sup>th</sup> Edition.
3. Chatwal, G.R. (2014). *Reaction Mechanism and Reagents in Organic Chemistry*. Mumbai: Himalaya Publishing House, 5<sup>th</sup> Edition.
4. Parmar & Chawla, (2001). *Reaction Mechanism in Organic Chemistry*. New Delhi: Sultan Chand & Sons, 2<sup>nd</sup> Edition.

### REFERENCE BOOKS

1. Eliel, E. Wilen, S.H. & Mander, L.N. (2008). *Stereochemistry of Organic Compounds*. New Jersey: John Wiley & Sons, 1<sup>st</sup> Edition.
2. Finar, I.L. (2003). *Organic Chemistry*. Vol. II, Singapore: Pearson Education, 5<sup>th</sup> Edition.
3. Nasipuri, D. (2004). *Stereochemistry of Organic Compounds*. New Delhi: New Age International (P) Ltd., 2<sup>nd</sup> Edition.
4. Kalsi, P.S. (2015). *Stereochemistry, Conformation and Mechanism*. New Delhi: New Age International Publishers, 8<sup>th</sup> Edition.
5. Jerry March, (2010). *Advanced Organic Chemistry*. New Jersey: John Wiley & Sons, 4<sup>th</sup> Edition.
6. Gould, E.S. (1959). *Mechanism and Structure in Organic Chemistry*. New York: Henry Holt & Co., 1<sup>st</sup> Edition.

Course Code 20PCHC21	PO1		PO2	PO3		PO4	PO5	PO6	PO7	PO8
	PSO 1.a	PSO 1.b	PSO 2	PSO 3.a	PSO 3.b	PSO 4	PSO 5	PSO 6	PSO 7	PSO 8
CO1	H	H	L	H	H	H	H	H	M	M
CO2	H	M	M	H	H	H	H	H	M	M
CO3	H	M	M	H	H	H	H	H	M	M
CO4	H	H	M	H	H	H	H	H	M	M
CO5	H	H	M	H	H	H	H	H	M	M

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**M.Sc. CHEMISTRY**  
**(2022-2023 onwards)**

Semester II	<b>STEREOCHEMISTRY AND REACTION MECHANISM</b>	Hours/Week: 6	
Core Course-4		Credits: 4	
Course Code 20PCHC21N		Internal 40	External 60

### COURSE OUTCOMES

On completion of the course, students will be able to

- CO1: describe prochirality and prostereoisomerism, the conformations of acyclic and Cyclic systems and the basic concepts of substitution, addition and elimination reactions. [K2]
- CO2: predict the nomenclature of prostereoisomers; interpret Cram and Prelog rules, Curtin - Hammett principle, neighboring group participation of n,  $\pi$  and  $\sigma$  electrons and the stereochemical factors in substitution, addition and elimination reactions. [K3]
- CO3: analyse the enantiotopic and diastereotopic ligands and faces, conformations of cyclohexanones, aldohexopyranoses and decalin and the mechanisms involved in substitution, addition and elimination reactions. [K4]
- CO4: correlate the optical isomerism in molecules with no chiral centers, conformations of acyclic and cyclic systems with their physical and chemical properties, nucleophilicity and basicity, electrophilic, nucleophilic and free radical additions and aromatic electrophilic and nucleophilic substitution reactions. [K4]
- CO5: categorize nucleophilic substitution at various carbon centers, electrophilic, nucleophilic and free radical additions to multiple bonds,  $\alpha$  - elimination,  $\beta$  - elimination and pyrolytic cis elimination reactions and stereospecific and stereoselective reactions. [K5]

**UNIT I Aliphatic nucleophilic substitution**

Nucleophilicity and basicity –  $S_N1$  and  $S_N2$  mechanisms – effect of substrate structure – effect of the attacking nucleophile – effect of the leaving group – effect of the reaction medium – ambident nucleophiles – ambident substrates – neighbouring group participation of  $n$ ,  $\pi$  and  $\sigma$  electrons –  $S_Ni$  mechanism – nucleophilic substitution at an aliphatic trigonal carbon – nucleophilic substitution at allylic carbon – nucleophilic substitution at vinyl carbon.

**Aliphatic electrophilic substitution:** Electrophilic substitution at saturated carbon  $S_{E1}$ ,  $S_{E2}$  mechanisms. (18 Hours)

**UNIT II Aromatic substitution and Elimination Reactions**

$\alpha$  - elimination -  $\beta$  - elimination -  $E1$ ,  $E2$  and  $E1cB$  mechanisms - stereochemistry of elimination - orientation of the double bond - effect of change in the substrate, base, leaving group and medium on  $E1$ ,  $E2$  and  $E1cB$  reactions - elimination vs substitution - pyrolytic eliminations - Bredt's rule.

Orientation - reactivity - mechanism of nitration, halogenation, Friedal - Craft's reaction and sulphonation - partial rate factors – ortho / para ratio - quantitative treatment of reactivity of the electrophile (the selectivity relationship) - Aromatic nucleophilic substitution reactions -  $S_{N1Ar}$ ,  $S_{N2}$  and benzyne mechanisms. (18 Hours)

**UNIT III Addition to multiple bonds**

Electrophilic, nucleophilic and free radical additions - addition to conjugated systems - orientation of the addendum - stereochemical factors in reactions like addition of hydrogen, halogens, hydrogen halides and hypohalous acids hydroboration and hydroxylation – epoxidation. Addition to carbonyl groups - mechanism of Aldol condensation - Perkin reaction - Knoevenagel reaction –Mannich reaction- Cannizzaro reaction - Benzoin condensation - Claisen ester condensation - Darzen's reaction - Reformatsky reaction - Wittig reaction - Grignard reactions. Addition to  $\alpha$ ,  $\beta$  - Unsaturated carbonyl groups - Michael addition - Diels - Alder reaction - Esterification of acids and hydrolysis of esters.

(18 Hours)

**UNIT IV Stereochemistry II**

Prochirality and prostereoisomerism, enantiotopic and diastereotopic ligands and faces and their nomenclature - pro-R and pro-S and  $R_e$  and  $S_i$  faces. Stereospecific and stereoselective reactions. Asymmetric synthesis: Cram and Prelog rules. Determination of enantiomeric and diastereomeric excess; enantio-discrimination. Optical isomerism due to

axial chirality - biphenyls, allenes and spiranes. Molecules with planar chirality - paracyclophanes, trans-cyclooctene, ansa compounds. (18 Hours)

### UNIT V Conformational analysis

Configuration and conformation - conformations of ethane and n-butane - conformational analysis - stereoelectronic and steric factors - conformation of simple acyclic compounds - conformation of monosubstituted and disubstituted cyclohexanes - correlation of the conformation of acyclic and cyclic systems with their physical and chemical properties - conformational free energy - Curtin - Hammett principles - Quantitative treatment of mobile system - Eliel-Ro equation- conformations and reactivity of cyclohexanones - conformational analysis of aldohexopyranoses-conformation of fused ring system-decalin- conformational effects in medium sized rings –concept of I strain. (18 Hours)

### TEXT BOOKS

1. Ahluwalia, V.K. (2015). *Organic Reaction Mechanism*. New Delhi: Narosa Publishing House, 4<sup>th</sup> Edition.
2. Chatwal, G.R. (2014). *Reaction Mechanism and Reagents in Organic Chemistry*. Mumbai: Himalaya Publishing House, 5<sup>th</sup> Edition.
3. Parmar & Chawla, (2001). *Reaction Mechanism in Organic Chemistry*. New Delhi: Sultan Chand & Sons, 2<sup>nd</sup> Edition.
4. Ramesh, P. (2005). *Basic Principles of Organic Stereochemistry*. Madurai: Meenu Publishers, 1<sup>st</sup> Edition.

### REFERENCE BOOKS

1. Finar, I.L. (2003). *Organic Chemistry*. Vol.II, Singapore: Pearson Education, 5<sup>th</sup> Edition.
2. Nasipuri, D. (2004). *Stereochemistry of Organic Compounds*. New Delhi: New Age International (P) Ltd., 2<sup>nd</sup> Edition.
3. Jerry March, (2010). *Advanced Organic Chemistry*. New Jersey: John Wiley & Sons, 4<sup>th</sup> Edition.
4. Gould, E.S. (1959). *Mechanism and Structure in Organic Chemistry*. New York: Henry Holt & Co., 1<sup>st</sup> Edition.
5. Eliel, E. Wilen, S.H. & Mander, L.N. (2008). *Stereochemistry of Organic Compounds*. New Jersey: John Wiley & Sons, 1<sup>st</sup> Edition.

6. Kalsi, P.S. (2015). *Stereochemistry, Conformation and Mechanism*. New Delhi: New Age International Publishers, 8<sup>th</sup> Edition.
7. Jonathan Clayden, Nick Greeves & Stuart Warren (2015), *Organic Chemistry*, Oxford University press Publishers, 2<sup>nd</sup> Edition.

Course Code 20PCHC21N	PO1		PO2	PO3		PO4	PO5	PO6	PO7	PO8
	PSO 1.a	PSO 1.b	PSO 2	PSO 3.a	PSO 3.b	PSO 4	PSO 5	PSO 6	PSO 7	PSO 8
CO 1	H	H	L	H	H	H	H	H	M	M
CO 2	H	M	M	H	H	H	H	H	M	M
CO 3	H	M	M	H	H	H	H	H	M	M
CO 4	H	H	M	H	H	H	H	H	M	M
CO 5	H	H	M	H	H	H	H	H	M	M

Dr. J.Kavitha

Head of the Department

Mrs.R.Nagasathya  
Mrs.A.Prasanna  
Dr. K.Malathi  
Course Designers



## V.V.VANNIAPERUMAL COLLEGE FOR WOMEN

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VIRUDHUNAGAR - 626 001

### M.Sc. CHEMISTRY

(For those who join in the Academic Year 2020-2021)

Semester II	<b>COORDINATION CHEMISTRY AND F-BLOCK ELEMENTS</b>	Hours/Week: 6	
Core Course-5		Credits: 5	
<b>Course Code 20PCHC22</b>		Internal 40	External 60

### COURSE OUTCOMES

On completion of the course, the students shall be able to

- CO1: understand the concepts involved in coordination compounds, polyacids, silicates, inorganic chains, rings, cages, f-block elements, photochemistry and electronic spectroscopy. [K2]
- CO2: predict the splitting pattern, stability and reactivity of co-ordination compounds, structure and bonding for inorganic compounds, properties and separation techniques in f-block elements, types of electronic transition and reactivity of complexes in photochemistry. [K3]
- CO3: apply LFT, CFT, MOT, Orgel, Tanabe – Sugano diagram and photo redox and substitution reactions for metal complexes, different techniques to identify the stability and reactivity of complexes, structure and bonding to identify the inorganic compounds, extraction techniques, spectral and magnetic behavior of f-block elements and [K3]
- CO4: analyze the structure, stability and reactivity of coordination and inorganic compounds, chemistry of f-block elements, Ru(II), Co(III) and Cr(III) complexes and different transitions involved in electronic spectrum. [K4]
- CO5: evaluate the structure, stability and reactivity of coordination and inorganic compounds, separation and characterization of f-block elements, electronic absorption spectrum of novel compounds and d-d transition in Ru(II), Co(III) and Cr(III) complexes. [K5]

**UNIT I Bonding in Coordination Compounds**

**CFT and LFT:** Basic features of CFT and LFT. Splitting of the metal *d*- orbitals in tetrahedral, octahedral and square planar symmetries –CFSE: Calculation of CFSE in octahedral and tetrahedral complexes –Factors affecting crystal field splitting- Spectral properties - Spectrochemical series - Magnetic properties of transition metal complexes- calculation of spin only magnetic moments- quenching of orbital magnetic moments– Kinetic properties.

**MOT:**  $\sigma$ -bonding and  $\pi$ -bonding in octahedral complexes - Effect of  $\pi$ -bonding on the value of  $\Delta(10Dq)$ . MOT for square planar (16  $e^-$ ) and tetrahedral (18  $e^-$ ) complexes. Application of MOT to spectrochemical series. (18 Hours)

**UNIT II Stability and Reactions of Co-ordination Compounds**

**Stability of complexes:** Thermodynamic and kinetic stabilities -stepwise and overall stability constants of the metal complexes – factors affecting stability – chelate and template effects - Determination of stability constants and composition of the complexes: Bjerrum's method, potentiometric determination, spectrophotometric method, ion-exchange method, polarographic method, continuous variation (Job's) method.

**Reactions of complexes:** Lability – inertness – Ligand substitution reactions of square planar complexes – Trans effect– Theories of trans effect – use of trans effect in synthesis of complexes– Substitution reactions in octahedral complexes – acid hydrolysis, base hydrolysis and anation reactions – Electron transfer reactions – Inner sphere and outer sphere processes– complementary and non-complementary reactions. (18 Hours)

**UNIT III Polyacids and Silicates**

**Polyacids:** classification – isopolyacids like polymolybdate, polyvanadate and polytungstate - structures – heteropolyacids 12A, 12B, 9 and 6 heteropolyacids – preparation and structures.

**Silicates:** various silicate structures and their properties.

**Inorganic Chains, Rings and Cages**

**Chains:** Catenation – (SN) systems –preparation, structure and bonding of silicones

**Rings:** Borazines and Phosphazines – preparation, structure, bonding and properties

**Cages:** Nomenclature of Boranes and carboranes – Wade's rule – styx number – preparation and structure of  $B_4H_{10}$ ,  $C_2B_{10}H_{12}$ ,  $(B_{12}H_{12})^{2-}$ . (18 Hours)

**UNIT IV LANTHANIDES AND ACTINIDES**

a) Lanthanides:- Occurrence- differences between 4f and 5f orbitals- position in the periodic table -Separation techniques (Fractional crystallisation, precipitation, ion-exchange, solvent-extraction and thermal decomposition- Selective reduction and oxidation)- Electronic configuration- Oxidation states, Lanthanide contraction- Spectral and Magnetic properties- Ln chelates-organometallic compounds of Ln. Uses of lanthanides (shift reagents, Pu bomb) and their compounds- aqueous chemistry of uranyl compounds.

b) Actinides:- - position in the periodic table - electronic configuration and oxidation states, spectral and magnetic properties- Synthesis of elements- Extraction of Th, U and Pu.

(18 Hours)

**UNIT V****a) Electronic absorption spectroscopy:**

Term symbols – selection rules – mechanism of breakdown of selection rules – band widths and shapes – Orgel diagrams – applications of Orgel diagrams to electronic spectra of transition metal complexes – charge transfer spectra – evaluation of  $10Dq$  and  $\beta$  for octahedral and tetrahedral complexes of  $d^3$ ,  $d^6$ ,  $d^7$ ,  $d^8$  configurations – effect of Jahn – Teller distortion on the electronic spectrum of complexes – Tanabe – Sugano diagram.

**b) Photochemistry of d-d transition and charge transfer transition**

Photoredox and photosubstitution reaction occurring in Ru(II), Co(III) and Cr(III) complexes.

(18 Hours)

**TEXT BOOKS**

1. Soni, P.L.(2016).*Coordination Chemistry*.New Delhi:Ane Books Pvt.Ltd.,1<sup>st</sup>Edition.
2. Gopalan, R.& Ramalingam, V. (2003).*Concise Coordination Chemistry*. New Delhi:Vikas Publishing House Pvt.Ltd.,1<sup>st</sup> Edition.
3. Sarkar, R. (2009).*General and Inorganic Chemistry*.New Delhi: New Central Book Agency, Pvt.Ltd.,1<sup>st</sup> Edition.
4. Mathur, H.D.& Tandon, O.P. (1989). *Chemistry of Rare Elements*. New Delhi: S. Chand and Company Ltd., 3<sup>rd</sup> Edition.
5. Rohatgi, K.K. & Mukherjee, (2018).*Fundamentals of Photo Chemistry*.New Delhi: New Age International Pvt.Ltd.,1<sup>st</sup> Edition.

**REFERENCE BOOKS**

1. Sathya Prakash, Tuli, G.D,Basu. S.K, Madan, R.D.(2008). *Advanced Inorganic Chemistry*.Volume - I , New Delhi: S.Chand & Company Ltd., 2<sup>nd</sup> Edition.

- Huheey, E. Ellen Keitler, A. & Richard Keitler, L. (2006). *Inorganic Chemistry*. New York: Dorling Kindersley Pvt. Ltd., 4<sup>th</sup> Edition.
- Cotton, F.A. & Wilkinson, G. (2007). *Advanced Inorganic Chemistry*. Singapore: John Wiley & sons, PTE Ltd., 6<sup>th</sup> Edition.
- Lee, J.D. (2007). *Concise Inorganic Chemistry*. Australia: Black Well Publishing Company, 5<sup>th</sup> Edition.

Course Code 20PCHC22	PO1		PO2	PO3		PO4	PO5	PO6	PO7	PO8
	PSO 1.a	PSO 1.b	PSO 2	PSO 3.a	PSO 3.b	PSO 4	PSO 5	PSO 6	PSO 7	PSO 8
CO1	H	H	H	H	H	M	H	H	H	M
CO2	H	H	M	H	H	H	H	H	H	M
CO3	H	H	M	H	H	H	H	M	H	M
CO4	H	H	H	H	H	H	H	M	H	M
CO5	H	H	H	H	H	H	H	M	H	M

Dr. J. Kavitha  
Head of the Department

Mrs. S.Lalithambigai  
Dr. M.Vairalakshmi  
Course Designers



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**VIRUDHUNAGAR - 626 001**

### M.Sc. CHEMISTRY

(2022-2023 onwards)

Semester II	<b>COORDINATION CHEMISTRY AND F-BLOCK ELEMENTS</b>	Hours/Week: 6	
Core Course-5		Credits: 5	
<b>Course Code</b> 20PCHC22N		Internal 40	External 60

### COURSE OUTCOMES

On completion of the course, the students shall be able to

- CO1: understand the concepts involved in coordination compounds, polyacids, silicates, inorganic chains, rings, cages, f-block elements and electronic spectroscopy. [K2]
- CO2: predict the splitting pattern, stability and reactivity of co-ordination compounds, structure and bonding for inorganic compounds, properties and separation techniques in f-block elements, inorganic chains, rings, cages types of electronic transition. [K3]
- CO3: apply LFT, CFT, MOT, Orgel, Tanabe – Sugano diagram, different techniques to identify the stability and reactivity of complexes, structure and bonding to identify the inorganic compounds, inorganic chains, rings, cages extraction techniques, spectral and magnetic behavior of f- block elements and [K3]
- CO4: analyze the structure, stability and reactivity of coordination and inorganic compounds, chemistry of f-block elements, inorganic chains, rings, cages and different transitions involved in electronic spectrum. [K4]
- CO5: evaluate the structure, stability and reactivity of coordination and inorganic compounds, separation and characterization of f-block elements, inorganic chains, rings, cages electronic absorption spectrum of novel compounds. [K5]

## UNIT I Bonding in Coordination Compounds

**CFT and LFT:** Basic features of CFT and LFT. Splitting of the metal  $d$ - orbitals in tetrahedral, octahedral and square planar symmetries – CFSE: Calculation of CFSE in octahedral and tetrahedral complexes – Factors affecting crystal field splitting- Spectral properties - Spectrochemical series - Magnetic properties of transition metal complexes- calculation of spin only magnetic moments- quenching of orbital magnetic moments– Kinetic properties.

**MOT:**  $\sigma$ -bonding and  $\pi$ -bonding in octahedral complexes - Effect of  $\pi$ -bonding on the value of  $\Delta(10Dq)$ . MOT for square planar ( $16 e^-$ ) and tetrahedral ( $18 e^-$ ) complexes. Application of MOT to spectrochemical series. (18 Hours)

## UNIT II Stability and Reactions of Co-ordination Compounds

**Stability of complexes:** Thermodynamic and kinetic stabilities - stepwise and overall stability constants of the metal complexes – factors affecting stability – chelate and template effects - Determination of stability constants and composition of the complexes: Bjerrum's method, potentiometric determination, spectrophotometric method, ion-exchange method, polarographic method, continuous variation (Job's) method.

**Reactions of complexes:** Lability – inertness – Ligand substitution reactions of square planar complexes – Trans effect– Theories of trans effect – use of trans effect in synthesis of complexes– Substitution reactions in octahedral complexes – acid hydrolysis, base hydrolysis and anation reactions – Electron transfer reactions – Inner sphere and outer sphere processes– complementary and non-complementary reactions. (18 Hours)

## UNIT III Electronic absorption spectroscopy:

LS coupling, Pigeon-Hole diagram - Term symbols – selection rules – mechanism of breakdown of selection rules – band widths and shapes – Orgel diagrams – applications of Orgel diagrams to electronic spectra of transition metal complexes – octahedral ( $d^3, d^6, d^7, d^8$ ) and tetrahedral complexes of ( $d^6, d^7, d^8$ ) configurations – evaluation of  $10Dq$  and  $\beta$  for octahedral ( $d^2, d^7$ ) and tetrahedral complexes of ( $d^7, d^8$ ) configurations using Tanabe – Sugano diagram- charge transfer spectra – Effect of John – Teller distortion on the electronic spectrum of complexes. (18 Hours)

**UNIT IV Polyacids and Silicates**

**Polyacids:** classification – isopolyacids like polymolybdate, polyvanadate and polytungstate - structures – heteropolyacids 12A, 12B, 9 and 6 heteropolyacids – preparation and structures.

**Silicates:** various silicate structures and their properties.

**Inorganic Chains, Rings and Cages**

**Chains:** Catenation – (SN) systems –preparation ,structure and bonding of silicones

**Rings:** Borazines and Phosphazines – preparation, structure,bonding and properties

**Cages:** Nomenclature of Boranes and carboranes – Wade’s rule – styx number – preparation and structure of  $B_4H_{10}$ ,  $C_2B_{10}H_{12}$ ,  $(B_{12}H_{12})^{2-}$ . (18 Hours)

**UNIT V LANTHANIDES AND ACTINIDES**

a) Lanthanides:- General features – occurrence –variable valencies -position in the periodic table -Separation techniques (Fractional crystallization, precipitation, ion-exchange, solvent-extraction and thermal decomposition- Selective reduction and oxidation)- Electronic configuration- Oxidation states, Lanthanide contraction- absorption spectra of Ln - magnetic properties- Ln chelates- Uses of lanthanides (shift reagents)

b) Actinides: General features – occurrence –variable valencies - electronic configuration and oxidation states, spectral and magnetic properties- trans actinide elements – chemistry of uranium – uranyl complexes – extraction cycles of U and Np. (18 Hours)

**TEXT BOOKS**

1. Soni, P.L.(2016).*Coordination Chemistry*.New Delhi:Ane Books Pvt.Ltd.,1<sup>st</sup>Edition.
2. Gopalan, R.& Ramalingam, V. (2003).*Concise Coordination Chemistry*. New Delhi:Vikas Publishing House Pvt.Ltd.,1<sup>st</sup> Edition.
3. Sarkar, R. (2009).*General and Inorganic Chemistry*.New Delhi: New Central Book Agency, Pvt.Ltd.,1<sup>st</sup> Edition.
4. Mathur, H.D.& Tandon, O.P. (1989). *Chemistry of Rare Elements*. New Delhi: S. Chand and Company Ltd., 3<sup>rd</sup> Edition

**REFERENCE BOOKS**

1. Sathya Prakash, Tuli, G.D, Basu. S.K, Madan, R.D.(2008). *Advanced Inorganic Chemistry*. Volume - I , New Delhi: S.Chand & Company Ltd., 2<sup>nd</sup> Edition.
2. Huheey, E. Ellen Keitler, A. & Richard Keitler, L. (2006). *Inorganic Chemistry*. New York: Dorling Kindersley Pvt. Ltd., 4<sup>th</sup> Edition.
3. Cotton, F.A.& Wilkinson, G. (2007). *Advanced Inorganic Chemistry*. Singapore: John Wiley & sons, PTE Ltd., 6<sup>th</sup> Edition.
4. Lee, J.D. (2007). *Concise Inorganic Chemistry*. Australia: Black Well Publishing Company, 5<sup>th</sup> Edition.
5. Puri B.R, Sharma L. R, Kalia K.C (2007). *Principles of Inorganic Chemistry*. Milestone Publishers & Distributors, 1<sup>th</sup> Edition.
6. Simon Cotton, *Lanthanide and Actinide Chemistry*, John Wiley & Sons, Ltd. 2006.

Course Code 20PCHC22N	PO1		PO2	PO3		PO4	PO5	PO6	PO7	PO8
	PSO 1.a	PSO 1.b	PSO 2	PSO 3.a	PSO 3.b	PSO 4	PSO 5	PSO 6	PSO 7	PSO 8
CO 1	H	H	H	H	H	M	H	H	H	M
CO 2	H	H	M	H	H	H	H	H	H	M
CO 3	H	H	M	H	H	H	H	M	H	M
CO 4	H	H	H	H	H	H	H	M	H	M
CO 5	H	H	H	H	H	H	H	M	H	M

Dr. J. Kavitha

Head of the Department

Dr. C. Vidya Rani  
Dr. M. Vairalakshmi

Course Designers



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**VIRUDHUNAGAR - 626 001**

**M.Sc. CHEMISTRY**

**(For those who join in the Academic Year 2020-2021)**

Semester II	<b>GROUP THEORY, STATISTICAL THERMODYNAMICS AND MACROMOLECULAR CHEMISTRY</b>	Hours/Week: 6	
Core Course-6		Credits: 5	
Course Code <b>20PCHC23</b>		Internal 40	External 60

**COURSE OUTCOMES**

On completion of the course, the students shall be able to

- CO1: discuss the basic concepts of Group theory, statistical and non equilibrium thermodynamics. [K2]
- CO2: predict ensemble averaging, thermodynamic properties of partition functions, heat capacity behavior of solids, entropy production and types and properties of polymers. [K3]
- CO3: apply the concepts of Group theory to spectroscopy and predict Huckel molecular orbital theory. [K3]
- CO4: calculate kinetics and mechanism for synthesis of macromolecules and develop procedure for molecular weight determination of macromolecules, construct the character Tables using Great Orthogonality theorem and identify relation of irreversible thermodynamics with biological systems. [K4]
- CO5: develop applications of HMO theory, Onsager's reciprocal theory, partition functions and new polymers in material science. [K5]

**UNIT I**

**GROUP THEORY**

Molecular symmetry elements and symmetry operations – vector and matrix algebra – symmetry operations and transformation matrices – Group definition and properties of a group – Symmetry point groups – Representation of a group – reducible and irreducible

representations – Great Orthogonality theorem – Characters – construction of character tables  
–  $C_{2v}$ ,  $C_{3v}$  – Direct Product concept. (18 Hours)

## UNIT II

### Application of group theory to spectroscopy and molecular problems:

Symmetry of normal modes of vibrations, Application of group theory to normal modes of vibrations and to normal mode analysis – symmetry properties of integrals – application for spectral selection rules of vibration spectra – IR and Raman active fundamentals ( $NH_3$ ,  $BF_3$ ) – Mutual Exclusion principle - Symmetry of molecular orbital symmetry selection rule for electronic transitions in simple molecules like ethylene, formaldehyde – Group theory and quantum mechanics – Wave functions as the basis of irreducible representation – group theory applied to hybridization – HMO theory – HMO calculations of delocalization energy for cyclopropenyl, butadiene, benzene. (18 Hours)

## UNIT III

### STATISTICAL THERMODYNAMICS

Concept of distribution, Thermodynamic probability and entropy, Maxwell-Boltzmann most probable distribution – Ensemble averaging – Postulates of ensemble averaging – Canonical – Grand canonical and microcanonical ensembles.

Partitions functions – translational, rotational vibrational and electronic partition functions – calculation of thermodynamic properties in terms of partition functions – Applications of partition functions.

Heat capacity behavior of solids – Chemical equilibria and Equilibrium constant in terms of partition functions - Fermi-Dirac statistics, Bose-Einstein's statistics. (18 Hours)

## UNIT IV

### NON-EQUILIBRIUM THERMODYNAMICS:

Introduction – Conservation of mass and energy – Entropy production – Entropy production in chemical reactions – Entropy production and entropy flow in open systems – Transformation properties of rates and affinities – Onsager's theory – validity of Onsager equation and its verification – The principle of microscopic reversibility and Onsager reciprocal relations – Transference in aqueous solutions of electrolytes – Stationary non-equilibrium states – Irreversible thermodynamics and biological systems – Irreversible thermodynamics for non-linear regime. (18 Hours)

**UNIT V****MACROMOLECULES:**

Types and properties of polymers – Kinetics and mechanism of free radical, ionic condensation and Ziegler-Natta polymerization processes – Emulsion and Suspension polymerization techniques – Polymer molecular weight and its distribution – Molecular weight determination – Osmotic pressure method – light scattering method – ultracentrifuge method – viscosity method. New polymers in material science – conducting polymers.

(18 Hours)

**TEXT BOOKS**

1. Ramakrishnan, V. & Gopinath, (2013). *Group Theory in Chemistry*. New Delhi: Vishal Publications, 2<sup>nd</sup> Edition.
2. Raman, K.V. (1990). *Group Theory and Its Applications to Chemistry*. New York: Tata McGraw-Hill Publishing Company, 1<sup>st</sup> Edition.
3. Bhattacharya, P.K. (2010). *Group Theory and Its Chemical Applications*. Mumbai: Himalaya Publishing House, 1<sup>st</sup> Edition.
4. Puri, B.R. Sharma, L. R. and Pathania, M.S. (2003). *Principles of Physical Chemistry*. New Delhi: Vishal Publishing Co, 1<sup>st</sup> Edition.
5. Gurdeep Raj, S. (2003). *Advanced Physical Chemistry*. Meerut: Goel Publishing Co. 25<sup>th</sup> Edition.
6. Bajpai, D.N. (2011). *Advanced Physical Chemistry*. New Delhi: S.Chand & Co., Ltd., 1<sup>st</sup> Edition.
7. Rajaram, J. & Kuriakose, J.C. (2003). *Thermodynamics*. New Delhi: Shoban Lal Nagin, Chand & Co., Ltd., 3<sup>rd</sup> Edition.
8. Glasstone, S. (2008). *Thermodynamics for Chemists*. New Delhi: East-West Press (P) Ltd., 1<sup>st</sup> Edition.
9. Gowariker, V.R. Viswanathan, N.V. and Sreedhar, J. (2001). *Polymer Science*. New Delhi: Wiley Eastern Ltd., 1<sup>st</sup> Edition.

**REFERENCE BOOKS**

1. Cotton, F.A. (2016). *Chemical Applications of Group Theory*. New York: John Wiley & Sons, 3<sup>rd</sup> Edition.
2. Salahuddin Kunju, A., Krishnan, G. (2015). *Group Theory and Its Application in Chemistry*. Delhi: PHI Learning Pvt. Ltd., 3<sup>rd</sup> Edition.
3. Atkins, P.W. (2002). *Physical Chemistry*. New York: ELPS and Oxford University Press, 4<sup>th</sup> Edition.

4. Billmeyer.F.W,(2001). *Text Book of Polymer Science*. New York: Wiley Interscience Publishers, 3<sup>rd</sup>Edition.

Course Code 20PCHC23	PO1		PO2	PO3		PO4	PO5	PO6	PO7	PO8
	PSO 1.a	PSO 1.b	PSO 2	PSO 3.a	PSO 3.b	PSO 4	PSO 5	PSO 6	PSO 7	PSO 8
CO1	H	M	M	H	H	H	H	M	H	L
CO2	H	M	H	H	H	H	H	M	H	L
CO3	H	M	H	H	H	H	H	H	H	L
CO4	H	M	H	H	H	H	H	H	H	L
CO5	H	M	H	H	H	H	H	H	H	L

Dr. J. Kavitha  
Head of the Department

Dr.J.Kavitha  
Dr.A.Anitha  
Course Designers



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VIRUDHUNAGAR - 626 001

### M.Sc. CHEMISTRY (2022-2023 onwards)

Semester II	<b>GROUP THEORY, STATISTICAL AND NON-EQUILIBRIUM THERMODYNAMICS</b>	Hours/Week: 6	
Core Course-6		Credits: 5	
Course Code <b>20PCHC23N</b>		Internal 40	External 60

#### COURSE OUTCOMES

On completion of the course, the students shall be able to

- CO1: discuss the basic concepts of Group theory, statistical and non equilibrium thermodynamics. [K2]
- CO2: predict ensemble averaging , thermodynamic properties of partition functions, heat capacity behavior of solids, entropy production and types and linear laws of non-equilibrium thermodynamics.. [K3]
- CO3: apply the concepts of Group theory to spectroscopy and predict Huckel molecular orbital theory and statistical & non-equilibrium thermodynamics [K3]
- CO4: construct the character Tables using Great Orthogonality theorem and identify relation of irreversible thermodynamics with biological systems. [K4]
- CO5: develop applications of HMO theory, Onsager's reciprocal theory, partition functions and statistical & non-equilibrium thermodynamics. [K5]

#### UNIT I GROUP THEORY

Group definition and properties of a group - Molecular symmetry elements and symmetry operations – vector and matrix algebra – symmetry operations and transformation matrices — Symmetry point groups – Representation of a group – reducible and irreducible representations – Great Orthogonality theorem – Characters – construction of character tables –  $C_{2v}$ ,  $C_{3v}$  – Direct Product concept. (18 Hours)

## **UNIT II Application of group theory to spectroscopy and molecular problems:**

Symmetry of normal modes of vibrations, Application of group theory to normal modes of vibrations and to normal mode analysis – symmetry properties of integrals – application for spectral selection rules of vibration spectra – IR and Raman active fundamentals (NH<sub>3</sub>, BF<sub>3</sub>) – Mutual Exclusion principle - Symmetry of molecular orbital symmetry selection rule for electronic transitions in simple molecules like ethylene, formaldehyde – Group theory and quantum mechanics – Wave functions as the basis of irreducible representation – group theory applied to hybridization – HMO theory – HMO calculations of delocalization energy for cyclopropenyl, butadiene, benzene.

(18 Hours)

## **UNIT III**

### **STATISTICAL THERMODYNAMICS**

Concept of distribution, Thermodynamic probability and entropy, Maxwell-Boltzmann most probable distribution – Ensemble averaging – Postulates of ensemble averaging – Canonical – Grand canonical and microcanonical ensembles.

Partitions functions – translational, rotational vibrational and electronic partition functions – calculation of thermodynamic properties in terms of partition functions – Applications of partition functions.

Heat capacity behavior of solids – Chemical equilibria and Equilibrium constant in terms of partition functions - Fermi-Dirac statistics, Bose-Einstein's statistics. (18 Hours)

## **UNIT IV**

### **NON-EQUILIBRIUM THERMODYNAMICS - I:**

Introduction – Conservation of mass and energy – Entropy production – Entropy production in heat flow, Entropy production in chemical reaction, Entropy production and entropy flow in open system – Forces and fluxes – Phenomenological Laws and Onsager Reciprocal Relations – Principle of microscopic reversibility and Onsager Reciprocal relation. (18 Hours)

## **UNIT V**

### **NON-EQUILIBRIUM THERMODYNAMICS - II:**

Wiener-Khintchine Theorem –Linear laws - Transformation properties of rates and affinities- Transference in aqueous solutions of electrolytes – Stationary non-equilibrium states – Irreversible thermodynamics to biological systems – Non-linear thermodynamics of irreversible process. (18 Hours)

**TEXT BOOKS**

1. Ramakrishnan, V. & Gopinath, (2013). *Group Theory in Chemistry*. New Delhi: Vishal Publications, 2<sup>nd</sup> Edition.
2. Raman, K.V. (1990). *Group Theory and Its Applications to Chemistry*. New York: Tata McGraw-Hill Publishing Company, 1<sup>st</sup> Edition.
3. Swarnalakshmi, S, Saroja, T, & Ezhilarasi, R.M. (2000), *A Simple Approach to Group Theory in Chemistry*, Universities Press, 3<sup>rd</sup> Edition.
4. Bhattacharya, P.K. (2010). *Group Theory and Its Chemical Applications*. Mumbai: Himalaya Publishing House, 1<sup>st</sup> Edition.
5. Puri, B.R. Sharma, L. R. and Pathania, M.S. (2003). *Principles of Physical Chemistry*. New Delhi: Vishal Publishing Co, 1<sup>st</sup> Edition.
6. Gurdeep Raj, S. (2003). *Advanced Physical Chemistry*. Meerut: Goel Publishing Co. 25<sup>th</sup> Edition.
7. Bajpai, D.N. (2011). *Advanced Physical Chemistry*. New Delhi: S.Chand & Co., Ltd., 1<sup>st</sup> Edition.
8. Rajaram, J. & Kuriakose, J.C. (2003). *Thermodynamics*. New Delhi: Shoban Lal Nagin, Chand & Co., Ltd., 3<sup>rd</sup> Edition.
9. Glasstone, S. (2008). *Thermodynamics for Chemists*. New Delhi: East-West Press (P) Ltd., 1<sup>st</sup> Edition.

**REFERENCE BOOKS**

1. Cotton, F.A. (2016). *Chemical Applications of Group Theory*. New York: John Wiley & Sons, 3<sup>rd</sup> Edition.
2. Salahuddin Kunju, A., Krishnan, G. (2015). *Group Theory and Its Application in Chemistry*. Delhi: PHI Learning Pvt. Ltd., 3<sup>rd</sup> Edition.
3. Atkins, P.W. (2002). *Physical Chemistry*. New York: ELPS and Oxford University Press, 4<sup>th</sup> Edition.

Course Code 20PCHC23N	PO1		PO2	PO3		PO4	PO5	PO6	PO7	PO8
	PSO 1.a	PSO 1.b	PSO 2	PSO 3.a	PSO 3.b	PSO 4	PSO 5	PSO 6	PSO 7	PSO 8
CO 1	H	M	M	H	H	H	H	M	H	M
CO 2	H	M	H	H	H	H	H	M	H	M
CO 3	H	M	H	H	H	H	H	H	H	M
CO 4	H	M	H	H	H	H	H	H	H	M
CO 5	H	M	H	H	H	H	H	H	H	M

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Course Designers



*Curriculum for M.Sc., Chemistry*

**V.V.VANNIAPERUMAL COLLEGE FOR WOMEN**  
(Belonging to Virudhunagar Hindu Nadars)  
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**VIRUDHUNAGAR - 626 001**

**M.Sc. CHEMISTRY**  
**(For those who join in the Academic Year 2020-2021)**

Semester II	<b>Inorganic Qualitative Analysis and Complex metric Titrations with EDTA</b>	Hours/Week: 6	
Core Practical-2		Credits: 3	
Course Code <b>20PCHC21P</b>		Internal 40	External 60

### **COURSE OUTCOMES**

On completion of the course, the students shall be able to

- CO1: apply systematic procedure and find out the familiar cations present in the given mixture of salts. [K3]
- CO2: apply systematic procedure and find out the less familiar cations present in the given salt mixture. [K3]
- CO3: calculate the amount of Nickel ions present in the given solution by direct and indirect EDTA volumetric methods. [K3]
- CO4: examine the amount of metal ions such as like Zinc, Magnesium and Copper present in the given solution by EDTA volumetric method and compare the result with the standard solution. [K4]
- CO5: develop the laboratory skill to deduce any unknown metal ions both by quantitative and qualitative analysis. [K5]

#### **I Semi – micro qualitative analysis:**

Analysis of mixtures containing two less familiar cations and two familiar cations from the following:

W, Se, Te, Mo, Ce, Zr, V and Li, Pb, Bi, Cu, Ni, Mn, Ba, Cd, Mg, Zn, Sr (Eight Mixtures)

#### **II. COMPLEXOMETRIC TITRATIONS WITH EDTA**

1. Estimation of ZINC
2. Estimation of MAGNESIUM
3. Estimation of COPPER
4. Estimation of NICKEL a) By Direct Method b) By Indirect Method

Course Code 20PCHC21P	PO1		PO2	PO3		PO4	PO5	PO6	PO7	PO8
	PSO 1.a	PSO 1.b	PSO2	PSO 3.a	PSO 3b	PSO 4	PSO 5	PSO 6	PSO 7	PSO 8
CO1	H	M	M	H	H	H	H	M	H	M
CO2	H	M	H	H	H	H	H	M	H	M
CO3	H	M	H	H	H	H	H	M	H	M
CO4	H	M	H	H	H	H	H	M	H	M
CO5	H	M	H	H	H	H	H	M	H	M

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Head of the Department

Dr.J.Kavitha  
Dr.M.Vairalakshmi  
Course Designers



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**VIRUDHUNAGAR - 626 001**

**M.Sc. CHEMISTRY**

(For those who join in the Academic Year 2020-2021)

Semester II	<b>ANALYTICAL CHEMISTRY</b>	Hours/Week: 6	
Discipline Specific Elective Course-2		Credits: 5	
Course Code <b>20PCHE21</b>		Internal 40	External 60

**COURSE OUTCOMES**

On completion of the course, the students will be able to

- CO1: understand the properties of precipitates, error analysis, types of electrodes, thermoanalytical and spectroanalytical methods. [K2]
- CO2: illustrate the methods of precipitation, statistical treatment of data, theory of electro analytical methods, principles of TGA, DSC, DTA, nephelometry, turbidimetry and flame spectrometry. [K3]
- CO3: interpret the calibration of instruments, different types of precipitations, reliability of results, and instrumentation of electroanalytical techniques, thermoanalytical methods, colorimetric and spectrophotometric analysis of elements. [K3]
- CO4: analyze the co-precipitation, post-precipitation, gravimetric analysis, error and statistical data, means of the two samples, determination of ions by electroanalytical methods, thermal behavior of various compounds and determination of metals by spectroanalytical methods. [K4]
- CO5: summarize the steps involved in gravimetric analysis, calibration of instruments, classification of errors, comparison of results, comparison of means of two samples and principle, instrumentation, applications of electroanalytical, thermoanalytical methods, and spectroanalytical methods for project. [K5]

### **UNIT I Precipitation Techniques**

Introduction- Properties of precipitates and precipitating reagents- Colloidal precipitates- Co-precipitation – Post-precipitation – Precipitation from homogeneous solution- Selective and Specific precipitation - Surface adsorption – Drying and ignition of precipitates – gravimetric analysis – principles – steps involved – calibration of instruments – burette and pipette calibration. (18 Hours)

### **UNIT II Error Analysis**

Error analysis: Classification of errors- accuracy and precision- minimization of errors- significant figures- significant figures in computation- statistical treatment of data: mean, median, standard deviations, variance, relative standard deviations- spread errors- standard deviation of computed results- reliability of results- Q-test, T -test, confidence limit-comparison of results- Student's t-test- F-test- comparison of means of the two samples- correlation and regression: linear regression (least square analysis) (18 Hours)

### **UNIT III Electroanalytical methods**

Electroanalytical Techniques: Electrogravimetry: Instrumentation - Theory of electrogravimetric analysis- electrolytic separation and determination of metal ions. Coulometry: Instrumentation - Electrolytic cell-working electrodes- auxillary electrode and reference electrode, electrode-coulometric titrations. Voltammetry –Principle, Instrumentation and applications of Cyclic voltammetry - stripping voltammetry - Amperometry: Amperometric titrations. (18 Hours)

### **UNIT IV Thermo analytical methods:**

Thermal analysis: Theory, Instrumentation and principles of DTA and TGA- factors affecting the position of DT and TG traces- application of DTA and TGA to the thermal behavior of the following compounds- crystalline copper sulphate, calcium oxalate monohydrate, calcium acetate monohydrate, ammonium nitrate, potassium chlorate with and without catalyst, ammonium Metavanadate, Zinc hexafluosilicate- complementary nature of DTA and TGA- principle, Instrumentation and applications of DSC- determination of degree of conversion of high alumina cement- purity determination- phase transition study- in forensic laboratory. (18 Hours)

**UNIT V Spectroanalytical Methods:**

Colorimetry: Beer and Lambert's law- terminology- condition for a satisfactory colorimetric analysis- methods of colour measurement or comparison- principles of colorimetric determinations of NH<sub>3</sub>, Cr, Cu, Fe, Mn- simultaneous spectrophotometric determination of Cr and Mn. Nephelometry and turbidimetry: principle- determination of sulphate and phosphate- fluorimetry: principle- application of fluorimetry in the determination of Cd, Ca and Zn and determination of codeine and morphine in a mixture. Flame spectrometry: - theory- interferences-AAS-applications in the determination of Mg<sup>2+</sup> and Ca<sup>2+</sup> in tap water, V in lubrication oil, trace lead in ferrous alloy and trace elements in contaminated soil.

(18 Hours)

**TEXT BOOKS**

1. Skoog,D.A., West,D.M. and Hollar.F.J,(2014). *Fundamentals of Analytical Chemistry*.U.K: Harcourt College Publishers, 9<sup>th</sup> Edition.
2. Usharani,S. (2000). *Analytical Chemistry*.Chennai: Macmillan India Ltd, 1<sup>st</sup> Edition.
3. Srivastava, A.K &Jain.P.C. (2009). *Instrumental Approach to Chemical Analysis*. New Delhi: S.Chand & Company Ltd., 4<sup>th</sup> Edition.

**REFERENCE BOOKS**

1. Gopalan,R., Subramanian,P.S., Rengarajan,K. (2016). *Elements of Analytical Chemistry*. New Delhi: Sultan Chand & Sons., 1<sup>st</sup> Edition.
2. Sharma,B.K. (2015). *Instrumental Methods of Chemical Analysis*.New Delhi: Krishna Prakashan Media Pvt.Ltd., 30<sup>th</sup> Edition.
3. Ahluwalia,V.K. (2016). *Instrumental Methods of Chemical Analysis*. New Delhi: Ane Books Pvt.Ltd.,1<sup>st</sup> Edition.

Course Code 20PCHE21	PO1		PO2	PO3		PO4	PO5	PO6	PO7	PO8
	PSO 1.a	PSO 1.b	PSO 2	PSO 3.a	PSO 3.b	PSO 4	PSO 5	PSO 6	PSO 7	PSO 8
CO1	H	H	L	H	H	H	H	M	M	L
CO2	H	H	L	H	H	H	H	M	M	L
CO3	H	H	L	H	H	H	H	M	M	L
CO4	H	H	L	H	H	H	H	M	M	L
CO5	H	H	L	H	H	H	H	M	M	L

Dr.J.Kavitha  
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Mrs.S.Lalithambigai  
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Course Designers



## V.V.VANNIAPERUMAL COLLEGE FOR WOMEN

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Re-accredited with 'A' Grade (3<sup>rd</sup> Cycle) by NAAC

**VIRUDHUNAGAR - 626 001**

### M.Sc. CHEMISTRY

(2022-2023 onwards)

Semester II	<b>ANALYTICAL CHEMISTRY</b>	Hours/Week: 6	
Discipline Specific Elective Course-2		Credits: 5	
Course Code <b>20PCHE21N</b>		Internal 40	External 60

#### COURSE OUTCOMES

On completion of the course, the students will be able to

CO1: Understand the concepts of error analysis, types of electrodes, thermoanalytical, electroanalytical, morphological techniques and spectroanalytical methods.[K2]

CO2: Illustrate statistical treatment of data, theory of electro analytical methods, principles of TGA, DSC, DTA, nephelometry, turbidimetry and flame spectrometry.[K3]

CO3: Interpret the calibration of instruments, reliability of results, and instrumentation of electroanalytical techniques, thermoanalytical methods, colorimetric and spectrophotometric analysis of elements.[K3]

CO4: Analyze error and statistical data, means of the two samples, determination of ions by electroanalytical methods, thermal behavior of various compounds and analysis by spectroanalytical, thermoanalytical, morphological techniques.[K4]

CO5: Summarize calibration of instruments, classification of errors, comparison of results, comparison of means of two samples and principle, instrumentation, applications of electroanalytical, thermoanalytical methods, morphological techniques and spectroanalytical methods for project. [K5]

#### UNIT I Error Analysis

Error analysis: Classification of errors- accuracy and precision- minimization of errors- significant figures- significant figures in computation- statistical treatment of data: mean, median, standard deviations, variance, relative standard deviations- spread errors- standard deviation of computed results- reliability of results- Q-test, T -test, confidence limit-

comparison of results- Student's t-test- F-test- comparison of means of the two samples- correlation and regression: linear regression (least square analysis) (18 Hours)

### **UNIT II Thermo analytical methods:**

Thermogravimetric Analysis: TGA apparatus, Factors affecting thermogram, Thermometric titrations-Applications of TGA-Determination of thermal stability of salts, Analysis of mixtures, Determination of Curie temperature.

Differential thermal Analysis: DTA apparatus, factors affecting DTA, Applications of DTA. Comparison of DTA and TGA thermograms.

Differential Scanning Calorimetry: Factors affecting DSC curve, Comparison of DTA and DSC techniques. (18 Hours)

### **UNIT III Electroanalytical methods**

Electroanalytical Techniques: Electrogravimetry: Instrumentation - Theory of electrogravimetric analysis- Applications of electrogravimetry. Coulometry: Instrumentation - coulometric titrations. Voltammetry –Principle, Instrumentation and applications of Cyclic voltammetry - stripping voltammetry - Amperometry: Amperometric titrations. Polarography- Polarograph and its working- Applications of polarography.

(18 Hours)

### **UNIT IV Morphological Techniques:**

**Scanning Electron Microscope:** Basic construction & its various parts. Working-Imaging techniques in SEM, secondary electron and back scattered electron- chemical analysis by energy dispersive X-ray analysis technique.

**Scanning Tunneling Microscope:** Principle, Instrumentation, working- piezo electric 3D scanner. Imaging methods: Constant current and constant height. Applications & limitations.

**Transmission Electron Microscope:** Principle, Instrumentation, working – sample preparation: powder and thin foil for TEM observation. Comparison of SEM & TEM.

**Atomic Force Microscopy:** Principle, Instrumentation, working – Applications of AFM.

(18 Hours)

### **UNIT V Spectroanalytical Methods:**

Colorimetry: Beer and Lambert's law- terminology- condition for a satisfactory colorimetric analysis- methods of colour measurement - principles of colorimetric determinations of Fe, Ni, composition of complexes.

Nephelometry and Turbidimetry: Theory and Instrumentation- Applications of Nephelometry and Turbidimetry.

Fluorimetry: Theory and instrumentation – factors affecting fluorimetric analysis - application of fluorimetry.

Flame photometry and Atomic Absorption spectroscopy: - Principle and instrumentation of flame photometer- AAS instrumentation and advantages. (18 Hours)

### TEXT BOOKS

4. Skoog,D.A., West,D.M. and Hollar.F.J,(2014). *Fundamentals of Analytical Chemistry*.U.K: Harcourt College Publishers, 9<sup>th</sup> Edition.
5. Usharani,S. (2000). *Analytical Chemistry*.Chennai: Macmillan India Ltd, 1<sup>st</sup> Edition.
6. Srivastava, A.K &Jain.P.C. (2009). *Instrumental Approach to Chemical Analysis*. New Delhi: S.Chand & Company Ltd., 4<sup>th</sup> Edition.

### REFERENCE BOOKS

1. Gopalan,R., Subramanian,P.S., Rengarajan,K. (2016). *Elements of Analytical Chemistry*. New Delhi: Sultan Chand & Sons., 1<sup>st</sup> Edition.
2. Sharma,B.K. (2015). *Instrumental Methods of Chemical Analysis*.New Delhi: Krishna Prakashan Media Pvt.Ltd., 30<sup>th</sup> Edition.
3. Ahluwalia,V.K. (2016). *Instrumental Methods of Chemical Analysis*. New Delhi: Ane Books Pvt.Ltd.,1<sup>st</sup> Edition.

Course Code 20PCHE21N	PO1		PO2	PO3		PO4	PO5	PO6	PO7	PO8
	PSO 1.a	PSO 1.b	PSO2	PSO3. a	PSO 3.b	PSO 4	PSO 5	PSO 6	PSO 7	PSO 8
CO 1	H	H	L	H	H	H	H	M	M	L
CO 2	H	H	L	H	H	H	H	M	M	L
CO 3	H	H	L	H	H	H	H	M	M	L
CO 4	H	H	L	H	H	H	H	M	M	L
CO 5	H	H	L	H	H	H	H	M	M	L

Dr.J.Kavitha  
Head of the Department

Dr. N.Ramiladevi  
Dr.M. Vairalakshmi  
Course Designers



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**VIRUDHUNAGAR - 626 001**

**M.Sc. CHEMISTRY**

**(For those who join in the Academic Year 2020-2021)**

Semester II	<b>POLYMER CHEMISTRY</b>	Hours/Week: 6	
Discipline Specific Elective Course-2		Credits: 5	
Course Code <b>20PCHE22</b>		Internal 40	External 60

**COURSE OUTCOMES**

On completion of the course, the students will be able to

- CO1: understand the classification of polymers. [K2]
- CO2: discuss the kinetics of polymerization techniques. [K2]
- CO3: illustrate the preparation of individual polymers. [K3]
- CO4: outline the properties of polymers and various techniques for processing polymers. [K4]
- CO5: evaluate the polymerization techniques, degradation and uses of polymers. [K5]

**UNIT I Classification of polymers and chemistry of polymerization**

Classification of polymers: Linear polymers, non-linear or branched polymers, cross-linked polymers, homo chain and hetero chain, homo polymers, co-polymers, block polymers and graft polymers.

Chemistry of polymerization: Types of polymerization—mechanism—chain, growth, free radical, ionic, co-ordination, ring opening, group transfer, poly addition and poly condensation polymerizations. (18 Hours)

**UNIT II Individual polymers**

Monomers required for general methods of preparation, repeat units and uses of the following polymers and resins – polyethylene, polystyrene, polyacrylonitrile, polymethylacrylate, PVC, polytetrafluoroethylene, polyisoprenes, polybutadienes and polychloroprene, polyesters, polycarbonates, polyimides, polyamides (Kelvar), polyurethanes,

polyethylene glycols, phenol-formaldehyde, urea-formaldehyde, melamine formaldehyde and epoxyresins– silicone polymers. (18 Hours) **UNIT**

### **III Properties of polymers**

Intrinsic properties–processing properties–article properties–basic idea of isomerism of polymers–configuration of polymer chain–geometrical structure–syndiotatic, isotatic and atatic polymers.

Glass transition temperature–Definition –factors affecting glass transition temperature–relationships between glass transition temperature and (a) molecular weight, (b) melting point and (c) plasticizer – importance of glass transition temperature– heat distortion temperature.

Molecular weight and size of polymers: Number average, weight average, sedimentation and viscosity average molecular weights–molecular weights and degree of polymerization– polydispersity–molecular weight distribution in polymers–size of polymer molecules– kinetics of polymerization. (18 Hours)

### **UNIT IV Polymerization techniques, degradation and uses of polymers**

Polymerization techniques: Bulk, solution, suspension, emulsion, melt condensation and interfacial polycondensation polymerizations.

Degradation: Types of degradation–thermal, mechanical, ultrasonic and photo degradation– photostabilizers–oxidative degradation–antioxidants–hydrolytic degradation. Uses of polymers in electronics and biomedicine. (18 Hours)

### **UNIT V Polymer processing**

Polymer processing – plastics (thermo and thermosetting), elastomers, fibres, compounding, plasticizers, colorants, flame retardants.

Compression and injection mouldings–film extrusion and calendaring–die casting and rotational casting– thermoforming– reinforcing. (18 Hours)

### **TEXT BOOKS**

1. Billmeyer, F.W.(2009). *Textbook of Polymer Science*. New Jersey: John Wiley and Sons, 3<sup>rd</sup> Edition.
2. Jain & Jain.(2013). *Engineering Chemistry*. New Delhi: Dhanpat Rai Publishing Company (P) Ltd, 16<sup>th</sup> Edition.
3. Jayashree Ghosh.(2013). *Fundamental Concepts of Applied Chemistry*. New Delhi:

S.Chand & Company Ltd, 1<sup>st</sup> Edition.

### REFERENCEBOOKS

1. Gowariker, V.R, Viswanathan, N.V. & Jayadev Sreedhar. (2009). *Polymer Science*. New Delhi: New Age International Publishers, 1<sup>st</sup> Edition.
2. Sharma.B.K,(1989). *Polymer Chemistry*. Meerut: Goel Publishing House, 1<sup>st</sup> Edition.
3. Bhatnagar. M.S. (2004). *A Text Book of Polymers* .Vol I, New Delhi: S.Chand & Company Ltd, 1<sup>st</sup> Edition.
4. Arora .M.G. Singh.M. (1996). *Polymer Chemistry*. New Delhi: Anmol Publications Pvt.Ltd., 1<sup>st</sup> Edition.
5. Davis.F.J. (2011). *Polymer Chemistry*. US:Oxford University Press.

Course Code 20PCHE22	PO1		PO2	PO3		PO4	PO5	PO6	PO7	PO8
	PSO 1.a	PSO 1.b	PSO 2	PSO 3.a	PSO 3.b	PSO 4	PSO 5	PSO 6	PSO 7	PSO 8
CO1	H	H	L	H	H	H	H	M	M	M
CO2	H	H	L	H	H	H	H	M	M	M
CO3	H	H	L	H	H	H	H	M	M	M
CO4	H	H	L	H	H	H	H	M	M	M
CO5	H	H	L	H	H	H	H	M	M	M

Dr. J. Kavitha  
Head of the Department

Dr.J.Kavitha  
Course Designer



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**M.Sc. CHEMISTRY**

**(For those who join in the Academic Year 2020-2021)**

Semester II	<b>INDUSTRIAL CHEMISTRY</b>	Hours/Week: 6	
Discipline Specific Elective Course-2		Credits: 5	
Course Code <b>20PCHE23</b>		Internal 40	External 60

**COURSE OUTCOMES**

On completion of the course, the students will be able to

CO1: understand the chemical concepts involved in dairy, leather and polymer products; chemistry involved in paint, pigments, energy resources and biofuels.

[K2]

CO2: acquire knowledge about the manufacturing processes of industrial products.

[K2]

CO3: analyse purity of industrial products. [K3]

CO4: apply the concept to harvest more energy from the natural resources and produce quality products. [K4]

CO5: prepare the novel industrial products. [K5]

**UNIT I**

**Dairy Chemistry**

Composition and structure of milk - milk lipids –fat globules –milk enzymes – vitamins – minerals - physical properties of milk –effect of heat –milk processing – clarification –pasteurization - homogenisation –milk products - cream, butter, ice cream, milk powder and ghee. (18 Hours)

**UNIT II**

**Leather Chemistry**

Introduction –structure of hide and skin –leather processing –process before tannage – flaying and curing –tanning process –methods of tanning –vegetable tanning –chrome tanning –aldehyde tanning –finishing processes after tanning –Tannery effluent and by – product problems –treatment of tanning wastes. (18 Hours)

**UNIT III****Polymer Chemistry**

History and significance of polymers- characteristics of polymers-Identification of polymers –polymers as adhesives –fillers –reinforcements-common plastic polymers used in packaging –PET,HDPE, PVC ,LDPE and PP-Revelation of polymer conductivity –doping – potential applications of conductivity polymers-polymers in lenses –biodegradable polymers-composition of biodegradable plastics –starch –based plastics –bacteria –based plastic – Soy –based plastics –biodegradable polyesters –PHA,PLA, PCL, PBS,AAC copolymers and modified PET –applications of biodegradable polymers –medical sutures, pins and dental implants. (18 Hours)

**UNIT IV****Pigments and Paints**

(a) White pigments –white lead, Zinc oxide, lithopone, titanium dioxide – characteristics and uses.

Blue pigments: ultra marine blue , cobalt blue and iron blue – characteristics & uses

Red pigments: Red lead, synthetic iron oxide - characteristics & uses

Green pigments: Chrome green, Reinmann’s green –uses.

(b)**Paints** : Requirements of a good paint –constituents of paint- manufacture of paints – emulsion paints –latex paints –varnishes –manufacture and uses –lacquers (18 Hours)

**UNIT V****Energy resources and Biofuels:-**

Chemical / Electrochemical and solar energy system- conventional and non – correctional energy resources, biomass and biochemical routes- hydrogen storage.

Biofuels-introduction, types of bio fuels (bioethanol and biodiesel)- raw materials for the synthesis of bio fuels, properties of bio fuels and the environment (Emissions from bio fuels),biofuels and economy, standard specification of biofuel, uses of biofuels – modification of vegetable oils as biodiesel. (18 Hours)

**TEXT BOOKS**

1. BK. Sharma, *Industrial Chemistry*, GOEL Publishing House, Meerut
2. K.Bagavathi Sundari, *Applied Chemistry*; MJP Publishers, Chennai,
3. Jayashree Ghosh, *Fundamental concepts of applied chemistry*, S.Chand &Company Ltd, Ram Nagar, New Delhi.

**REFERENCEBOOKS**

1. Dr. Vandana Meshram - Ingle, *A Textbook of Industrial Chemistry*, Educational Publisher and Distributors.
2. Raghunath B. Toche, Satish Kale, Eknath H. Gade, *A Textbook of Industrial Chemistry*, Vision Publications.

Course Code 20PCHE23	PO1		PO2	PO3		PO4	PO5	PO6	PO7	PO8
	PSO 1.a	PSO 1.b	PSO 2	PSO 3.a	PSO 3.b	PSO 4	PSO 5	PSO 6	PSO 7	PSO 8
CO1	H	H	L	H	H	H	H	M	M	M
CO2	H	H	L	H	H	H	H	M	M	M
CO3	H	H	L	H	H	H	H	M	M	M
CO4	H	H	L	H	H	H	H	M	M	M
CO5	H	H	L	H	H	H	H	M	M	M

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Course Designers



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VIRUDHUNAGAR - 626 001

### M.Sc. CHEMISTRY

(For those who join in the Academic Year 2020-2021)

Semester III	<b>ORGANIC SPECTROSCOPY, REARRANGEMENT, REAGENTS AND SYNTHETIC METHODS</b>	Hours/Week: 6	
Core Course-7		Credits: 4	
Course Code <b>20PCHC31</b>		Internal 40	External 60

### COURSE OUTCOMES

On completion of the course, students will be able to

- CO 1: precise the basic concepts of NMR Spectroscopy, pericyclic reactions, Oxidation and Reduction reactions, Rearrangements and Retrosynthetic analysis. [K2]
- CO 2: interpret the concepts of NMR to assign and ascertain the types of protons and carbon framework in organic compounds, mechanism of reactions and the usage of activating and blocking groups in synthesis. [K3]
- CO 3: identify <sup>1</sup>H NMR and <sup>13</sup>C NMR spectrum, the different approaches in pericyclic reactions, intermolecular and intramolecular mechanisms in rearrangements, the pathway of catalytic oxidation and reduction reactions and relay and convergent approaches to total synthesis. [K3]
- CO4: examine correlation spectrums and categorize photochemical reactions, molecular rearrangements, reagents in organic synthesis, stereoselective problems of geometrical and optical isomerism in planning a synthesis. [K4]
- CO 5: predict the factors affecting <sup>1</sup>H NMR and <sup>13</sup>C NMR, the stereochemical aspects of oxidation, reduction reactions and rearrangements, novel synthetic strategies in organic chemistry and justify the conservation of orbital symmetry in pericyclic reactions. [K5]

### UNIT I

#### Spectroscopy II:

<sup>1</sup>H NMR spectroscopy : Origin of NMR spectra– assignment of signal, relaxation time– chemical shift – coupling constant – first and second order spectra – spin-spin splitting – influence of stereochemical factors on chemical shift of protons – simplification of complex

spectra – deuterium substitution – spin decoupling – double resonance – shift reagents – Nuclear Overhauser Effect – CIDNP – NMR concept of aromaticity-H-H-COSY.

$^{13}\text{C}$  NMR spectroscopy: Introduction – Comparison of  $^{13}\text{C}$  NMR and  $^1\text{H}$  NMR spectroscopy – chemical shifts in  $^{13}\text{C}$  NMR and factors affecting  $^{13}\text{C}$  NMR – Off-resonance decoupling– calculation of chemical shifts for aromatic and aliphatic compounds – DEPT  $^{13}\text{C}$  spectra – HETCOR. (18 Hours)

## UNIT II

### Photochemistry

Conservation of orbital symmetry – electrocyclic reactions – cycloaddition reactions and sigmatropic rearrangements – applications of correlation diagram approach, Frontier molecular orbital approach, Huckel – Mobius approach and Perturbation molecular orbital approach to the above reactions.

Photochemical reactions of ketones – photosensitization – Norrish I and Norrish II type reactions – Paterno-Buchi reaction – photooxidation – photoreduction.

**Radical Initiated Reactions**-Barton, Sandmeyer, Gomberg-Bachmann, Pschorr, Ullmann, and Hundsdiecker reactions. (18 Hours)

## UNIT III

### Molecular rearrangements:

**Mechanism of the following rearrangement reactions** :Wagner-Meerwein, Pinacol-Pinacolone, Demjanov, Beckmann, Hofmann, Curtius, Wolff, Baeyer-Villegier, Stevens, Sommelet-Hauser, Favorskii, Benzil-benzilic acid, Claisen, Cope, Fries, Dienone-phenol, hydroxylamino-p-aminophenol, di- $\pi$  methane and benzidine rearrangement.

(18 Hours)

## UNIT IV

### Oxidation and Reduction:

Catalytic oxidation — mechanism, applications and stereo chemical aspects of the following oxidation reactions: Oxidation reaction involving  $\text{CrO}_3$ ,  $\text{SeO}_2$ ,  $\text{OsO}_4$ , lead tetraacetate, periodic acid, N-bromosuccinimide,  $\text{H}_2\text{O}_2$  – Oppenauer oxidation.

Catalytic reduction — mechanism, applications and stereochemical aspects of the following reduction reactions reaction involving lithiumaluminium hydride, triisobutylaluminium hydride, DIBAL and sodium borohydride – Birch reduction – Meerwin-Pondorf – Verley reduction – Wolf-Kishner reduction –hydroboration – selectivity in oxidation and reduction.

**Reagents in Organic synthesis**

Gilman's reagent (lithium dimethylcuparate), lithium diisopropylamide (LDA), Dicyclohexylcarbodiimide, 1,3 – dithiane, trimethylsilyl iodide, tri-n-butyltinhydride, Woodward and Prevost hydroxylation, DDQ, Merrifield resin, phase transfer catalysis, Peterson's synthesis, Baker's yeast. (18 Hours)

**UNIT V Retro Synthetic methods:**

Planning a synthesis – Relay approach and convergent approach to total synthesis – Retrosynthetic analysis of simple organic compounds – functional group interconversions – use of activating and blocking groups in synthesis – stereoselective problems of geometrical and optical isomerism – steric crowding – Transition metal complexes in organic chemistry – Homogeneous hydrogenation – Regioselectivity – Diastereoselectivity – Enantioselectivity – Umpolung synthesis – Robinson annelation – A schematic analysis of the total synthesis of the following compounds: 2,4-dimethyl-2-hydroxypentanoic acid, trans-9- methyl-1-decalone and isonootkatone.

(18 Hours)

**TEXT BOOKS**

1. Kalsi, P.S. (2014). *Spectroscopy of Organic Compounds*. New Delhi: New Age International Publishers, 6<sup>th</sup> Edition.
2. William Kemp. (2009). *Organic Spectroscopy*. New York: Palgrave, 3<sup>rd</sup> Edition.
3. Depuy. C.H. & Chapman, O.L. (1972). *Molecular Reactions and Photochemistry*. New Jersey: Prentice Hall, 1<sup>st</sup> Edition.
4. Chatwal, G.R. (2014). *Reaction Mechanism and Reagents in Organic Chemistry*. Mumbai: Himalaya Publishing House, 5<sup>th</sup> Edition.
5. Jagdamba Singh, Yadav, L.D.S. (2014). *Organic Synthesis*. Meerut: Pragati Prakashan, 1<sup>st</sup> Edition.
6. Finar, I.L. (2003). *Organic Chemistry*. Vol.II, Singapore: Pearson Education, 5<sup>th</sup> Edition.
7. Ireland, R.E. (1975). *Organic Synthesis*. New York: Prentice-Hall of India Pvt. Ltd., 1<sup>st</sup> Edition.

**REFERENCE BOOKS**

1. John Dyer, R.(2010). *Application of Absorption Spectroscopy of Organic Compounds*. New Delhi: PHI Learning Pvt. Ltd, 1<sup>st</sup> Edition .
2. Robert Silverstein, M. & Francis Webster, X. (2004). *Spectrometric Identification Organic Compounds*. New Jersey: John Wiley & Sons, Inc., 6<sup>th</sup> Edition.

3. Ratan Kumar Kar. (2008). *Fundamentals of Organic Synthesis*. Vol.II, New Delhi: New Central Book Agency Pvt.Ltd., 1<sup>st</sup> Edition.
4. Braithwaite, A. & Smith, F.J. (1985). *Chromatographic Methods*. London: Chapman and Hall, 4<sup>th</sup> Edition.
5. Agarwal O. P, *Organic Chemistry Reactions and Reagents*. Meerut: GOEL Publishing House, 22<sup>nd</sup> Edition
6. Sanyal S.N (2006), *Reactions, Rearrangements and Reagents*. Bangalore: Bharathi Bhawan Publishers and Distributors, 4<sup>th</sup> edition

Course Code 20PCHC31	PO1		PO2	PO3		PO4	PO5	PO6	PO7	PO8
	PSO 1.a	PSO 1.b	PSO 2	PSO3a	PSO 3.b	PSO 4	PSO 5	PSO 6	PSO 7	PSO 8
CO1	H	H	H	M	H	H	H	H	M	M
CO2	H	H	M	M	M	L	M	L	M	M
CO3	H	H	M	M	M	M	M	M	M	H
CO4	H	H	M	M	M	M	L	L	L	H
CO5	H	H	M	M	M	H	M	H	M	H

Dr. J. Kavitha  
Head of the Department

Mrs.R.Nagasathya  
Mrs.A.Prasanna  
Course Designers



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**VIRUDHUNAGAR - 626 001**

### M.Sc. CHEMISTRY

(2023-2024 onwards)

Semester III	<b>ORGANIC SYNTHESIS AND SPECTROSCOPY</b>	Hours/Week: 6	
Core Course-7		Credits: 4	
Course Code <b>20PCHC31N</b>		Internal 40	External 60

### COURSE OUTCOMES

On completion of the course, students will be able to

- CO 1: precise the basic concepts of NMR Spectroscopy, pericyclic reactions, Oxidation and Reduction reactions, Rearrangements and Retrosynthetic analysis.[K2]
- CO 2: interpret the concepts of NMR to assign and ascertain the types of protons and carbon framework in organic compounds, mechanism of reactions and the usage of activating and blocking groups in synthesis [K3]
- CO 3: identify <sup>1</sup>H NMR and <sup>13</sup>C NMR spectrum, the different approaches in pericyclic reactions, intermolecular and intramolecular mechanisms in rearrangements, the pathway of catalytic oxidation and reduction reactions and relay and convergent approaches to total synthesis [K3]
- CO4: examine correlation spectrums and categorize photochemical reactions, molecular rearrangements, reagents in organic synthesis, stereoselective problems of geometrical and optical isomerism in planning a synthesis. [K4]
- CO 5: predict the factors affecting <sup>1</sup>H NMR and <sup>13</sup>C NMR, the stereochemical aspects of oxidation, reduction reactions and rearrangements, novel synthetic strategies in organic chemistry and justify the conservation of orbital symmetry in pericyclic reactions. [K5]

### UNIT I

#### Photochemistry and Pericyclic reaction

Conservation of orbital symmetry – construction of molecular orbital and symmetry elements to simple molecules like 1,3-butadiene, 1,3,5-hexatriene, cyclobutene,

cyclohexadiene- electrocyclic reactions – cycloaddition reactions and sigmatropic rearrangements reactions– applications of FMO approach, Correlation approach-Huckel–Möbius approach-(dis- and con- rotatory ring closure of 1,3-butadiene, 1,3,5-hexatriene and  $(2\pi+2\pi)$ ,  $(4\pi+2\pi)$  cycloaddition reactions.

Photochemical reactions of ketones – photosensitization – Norrish I and Norrish II type reactions – Paterno-Buchi reaction – photo oxidation – photo reduction.

**Radical Initiated Reactions**-Barton, Sandmeyer, Gomberg - Bachmann, Pschorr, Ullmann, and Hunsdiecker reactions. (18 Hours)

## UNIT II

### Molecular rearrangements:

**Mechanism of the following rearrangement reactions** :Wagner-Meerwein, Pinacol-Pinacolone, Demjanov, Beckmann, Hofmann, Curtius, Wolff, Baeyer-Villiger, Stevens, Sommelet-Hauser, Favorskii, Benzil-benzilic acid, Claisen, Cope, Fries, Dienone-phenol, hydroxylamino-p-aminophenol, di- $\pi$  methane and benzidine rearrangement. (18 Hours)

## UNIT III

### Oxidation and Reduction:

Catalytic oxidation — mechanism, applications and stereo chemical aspects of the following oxidation reactions: Oxidation reaction involving  $\text{CrO}_3$ ,  $\text{SeO}_2$ ,  $\text{OsO}_4$ , lead tetraacetate, periodic acid, N-bromosuccinimide,  $\text{H}_2\text{O}_2$  – Oppenauer oxidation.

Catalytic reduction – mechanism, applications and stereochemical aspects of the following reduction reactions reaction involving lithiumaluminium hydride, triisobutylaluminium hydride, DIBAL and sodium borohydride – Birch reduction – Meerwin- Pondorf – Verley reduction – Wolf-Kishner reduction, Huang-Minon modification – hydroboration – selectivity in oxidation and reduction.

### Reagents

Gilman's reagent (lithium dimethylcuparate), lithium diisopropylamide (LDA), Dicyclohexylcarbodiimide, 1, 3 – dithiane, trimethylsilyl iodide, tri-n-butyltinhydride, Woodward and Prevost hydroxylation, DDQ, Merrifield resin, phase transfer catalysis, Peterson's synthesis, Baker's yeast. (18 Hours)

## UNIT IV Retro Synthesis:

Planning a synthesis – Relay approach and convergent approach to total synthesis – Retrosynthetic analysis of retrosynthetic analysis–carbon skeleton–functional group located on the skeleton–disconnection- C-X disconnection functional group interconversions – use of activating and blocking groups in synthesis – stereoselective problems of geometrical and

optical isomerism – steric crowding – Transition metal complexes in organic chemistry – Homogeneous hydrogenation – Regioselectivity – Diastereoselectivity – Enantioselectivity – Umpolung synthesis – Robinson annelation – A schematic analysis of the total synthesis of the following compounds: 2,4-dimethyl-2-hydroxypentanoic acid, trans-9-methyl-1-decalone and isonootkatone. (18 Hours)

## UNIT V

### Spectroscopy II:

$^1\text{H}$  NMR spectroscopy : Origin of NMR spectra– assignment of signal, relaxation time– chemical shift – coupling constant – first and second order spectra – spin-spin splitting – influence of stereochemical factors on chemical shift of protons – simplification of complex spectra – deuterium substitution – spin decoupling – double resonance – shift reagents – Nuclear Overhauser Effect – CIDNP – NMR concept of aromaticity-H-H-COSY.

$^{13}\text{C}$  NMR spectroscopy: Introduction – Comparison of  $^{13}\text{C}$  NMR and  $^1\text{H}$  NMR spectroscopy – chemical shifts in  $^{13}\text{C}$  NMR and factors affecting  $^{13}\text{C}$  NMR – Off-resonance decoupling–additivity relationship- calculation of chemical shifts for aromatic and aliphatic compounds – DEPT  $^{13}\text{C}$  spectra –  $^{13}\text{C}$  - $^{13}\text{C}$  correlation COSY, HETCOR ROESY, NOESY and TOCSY- Inadequate. (18 Hours)

### TEXT BOOKS

1. Depuy, C.H. & Chapman, O.L. (1972). *Molecular Reactions and Photochemistry*. New Jersey: Prentice Hall, 1<sup>st</sup> Edition.
2. Chatwal, G.R. (2014). *Reaction Mechanism and Reagents in Organic Chemistry*. Mumbai: Himalaya Publishing House, 5<sup>th</sup> Edition.
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	PSO 1.a	PSO 1.b	PSO 2	PSO3a	PSO 3.b	PSO 4	PSO 5	PSO 6	PSO 7	PSO 8
CO 1	H	H	H	M	H	H	H	H	M	M
CO 2	H	H	M	M	M	L	M	L	M	M
CO 3	H	H	M	M	M	M	M	M	M	H
CO 4	H	H	M	M	M	M	L	L	L	H
CO 5	H	H	M	M	M	H	M	H	M	H

Dr. J. Kavitha

Head of the Department

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Mrs. A. Prasanna  
Dr. K.Malathi  
Course Designers



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**M.Sc. CHEMISTRY**

**(For those who join in the Academic Year 2020-2021)**

Semester III	<b>ORGANOMETALLICS, NUCLEAR CHEMISTRY AND INORGANIC SPECTROSCOPY</b>	Hours/Week: 6	
Core Course - 8		Credits: 5	
Course Code <b>20PCHC32</b>		Internal 40	External 60

**COURSE OUTCOMES**

On completion of the course, the students will be able to

- CO1: understand the principle of spectroscopic techniques, nuclear and organometallic chemistry [K2].
- CO2: predict the nomenclature, stability, synthesis, structure, bonding, isolobal, isoelectronicity and catalytic behavior of organometallic compounds, nuclear reaction, forces, detectors, accelerators, application of radioactive substances, various compounds using spectroscopy techniques. [K3]
- CO3: apply the organometallic chemistry to synthesize industrial chemical reactions, nuclear chemistry to predict the radioactive substances and spectroscopic technique to study the structure of compounds. [K3].
- CO4: examine the stability, structure, bonding, synthesis and reactivity of organometallic compounds, isotopes, nuclear reaction and reactor and applications of EPR, NMR & NQR. [K4]
- CO 5: interpret the synthetic method, bonding, structural elucidation, stability and catalytic efficiency of organometallic compounds and spectral data. [K5]

**UNIT I ORGANOMETALLIC CHEMISTRY - I**

Organo metallic compounds- sixteen and eighteen electron rule - sigma, pi and haptic nomenclature – isoelectronic and isolobal analogy- Synthesis, structure and bonding of metal carbonyls, metal nitrosyls, dinitrogen complexes, Ferrocene, Arene complexes, olefin, acetylene and pi allyl complexes - use of IR in the structural elucidation of carbonyl compounds – pi donors-carboxylic ligands and complexes. (18 Hours)

**UNIT II ORGANOMETALLIC CHEMISTRY –II**

Oxidative addition and reductive elimination – insertion of alkenes and  $\beta$ -hydrogen elimination-Catalytic reactions- hydrogenation of olefins – Wilkinson's catalyst – hydroformylation – oxidation of olefins – Wacker process – propylene polymerization – Olefin metathesis -Ziegler Natta catalyst –cyclo oligomerisation of acetylene , butadiene- Reppe's catalyst . Mansanto's acetic acid synthesis-Fischer-Tropsch's synthesis of Synthetic gasoline. (18 Hours)

**UNIT III NUCLEAR CHEMISTRY**

Radioactive decay and equilibrium- Different types of nuclear reaction – spallation – fission and fusion. Theories of fission. Fissile and Fertile isotopes -Nuclear fusion – stellar energy-Nuclear forces: Liquid drop model, shell model-Calculation of Q-values – Cross section. Detectors: Scintillation counter, Gas ionisation chamber. Proportional Counter, Cerenkov Counter-Accelerators: Cyclotron, Synchrocyclotron, Betatron. Radio isotopes and their Applications: Activation analysis, Isotopic dilution technique-radiometric titration. Nuclear reactors: Types (Thermo nuclear and breeder reactors) feed materials production. Reprocessing of nuclear materials waste disposal. Atomic power projects in India. Hazardous of radioactive materials and Safety measures. (18 Hours)

**UNIT IV ESR Spectroscopy**

Principles – presentation of a spectrum – hyperfine splitting – evaluation of g tensor – Isotropy, Anisotropy in g value - factors affecting the magnitude of g – values – zero field splitting – Kramer's degeneracy – ESR of  $d^3$  octahedral complexes – anisotropy and hyper fine splitting constant – application of ESR in the study of transition metal complexes –  $VO^{2+}$ ,  $Fe^{3+}$ ,  $Co^{2+}$ ,  $Mn^{2+}$ ,  $Ni^{2+}$  and bisalicylaldimine copper (II) – Jahn Teller distortion studies in Cu (II) complexes. (18 Hours)

**UNIT V NMR AND NQR SPECTROSCOPY:****a) NMR Spectroscopy:**

Multinuclear NMR-  $^{31}P$ ,  $^{19}F$  and  $^{15}N$  NMR – introduction application in structural problem -  $ClF_3$ ,  $SF_4$ ,  $PF_5$ ,  $BrF_5$ ,  $P_4S_3$ ,  $PF_3(NH_2)_2$  - evaluation of rate constants –NMR of fluxional molecules –NMR of paramagnetic molecules- contact shifts and shift reagents.

### **b) NQR Spectroscopy:**

Introduction – effect of magnetic field on the spectra – relation between electric field gradient and structure – applications of NQR. (18 Hours)

### **TEXT BOOKS**

1. Gopalan, R. & Ramalingam, V. (2003). *Concise Coordination Chemistry*. New Delhi: Vikas Publishing House Pvt.Ltd., 1<sup>st</sup> Edition.
2. Arnikar, H.I. (2016). *Essentials of Nuclear Chemistry*. New Delhi: Wiley Eastern Ltd., 4<sup>th</sup> Edition.
3. Drago, R.S. (1977). *Physical Methods in Chemistry*. London: Saunders Golden Suburst Series, W.B.Saunders Company, 1<sup>st</sup> Edition.
4. Aruldas, G.(2013). *Molecular Structure and Spectroscopy*. New Delhi: PHI Learning Pvt.Ltd., 2<sup>nd</sup> Edition.

### **REFERENCE BOOKS**

1. Huheey, E. Keitler, A.& Keitler, L. (2006). *Inorganic Chemistry*. New York: Harper, Dorling Kindersley Pvt. Ltd., 4<sup>th</sup> Edition.
2. Shekar, C.V. (2014). *Nuclear Chemistry*. New Delhi: Dominant Publishers and Distributors Pvt. Ltd., 1<sup>st</sup> Edition.
3. Cotton, F.A. & Wilkinson, G. (2007). *Advanced Inorganic Chemistry*. Singapore: John, Wiley & Sons, 6<sup>th</sup> Edition.
4. Lee, J.D. (2007). *Concise Inorganic Chemistry*. Australia: Black Well Publishing Company, 5<sup>th</sup> Edition.
5. Soni, P.L. & PandnaSoni. (2016). *Coordination Chemistry*. New Delhi: Ane Books Pvt.Ltd., 1<sup>st</sup> Edition.

Course Code 20PCHC32	PO1		PO2	PO3		PO4	PO5	PO6	PO7	PO8
	PSO 1.a	PSO 1.b	PSO 2	PSO 3.a	PSO 3.b	PSO 4	PSO 5	PSO 6	PSO 7	PSO 8
CO1	H	H	M	H	H	M	H	H	M	M
CO2	H	H	M	H	H	M	H	H	M	M
CO3	H	H	L	H	H	M	H	H	L	M
CO4	H	H	L	H	H	M	H	H	L	M
CO5	H	H	M	H	H	M	H	H	M	M

Dr. J. Kavitha  
Head of the Department

Dr.M.Vairalakshmi  
Mrs. S. Lalithambigai  
Course Designers



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### M.Sc. CHEMISTRY

(2023-2024 onwards)

Semester III	<b>ORGANOMETALLICS, INORGANIC PHOTOCHEMISTRY AND SPECTROSCOPY</b>	Hours/Week: 6	
Core Course - 8		Credits: 5	
Course Code <b>20PCHC32N</b>		Internal 40	External 60

#### COURSE OUTCOMES

On completion of the course, the students will be able to

- CO1: understand the principle of spectroscopic techniques, photochemistry and organometallic chemistry [K2].
- CO2: predict the nomenclature, stability, synthesis, structure, bonding, isolobal, isoelectronicity and catalytic behavior of organometallic compounds, inorganic photochemistry and various compounds using spectroscopy techniques. [K3]
- CO3: apply the organometallic chemistry to synthesize industrial chemical reactions, Photochemical Unimolecular reactions and spectroscopic technique to study the structure of compounds.[K3].
- CO4: examine the stability, structure, bonding, synthesis and reactivity of Organometallic compounds, photochemical reactions of inorganic compounds and applications of EPR, NMR & NQR. [K4]
- CO 5: interpret the synthetic method, bonding, structural elucidation, stability and Catalytic efficiency of organometallic compounds, inorganic photochemical aspects and spectral data. [K5].

#### UNIT I ORGANOMETALLIC CHEMISTRY - I

Organo metallic compounds- sixteen and eighteen electron rule - sigma, pi and haptic nomenclature – isoelectronic and isolobal analogy- Synthesis, structure and bonding of metal carbonyls, metal nitrosyls, dinitrogen complexes, Ferrocene, Arene complexes, olefin, acetylene and pi allyl complexes - use of IR in the structural elucidation of carbonyl compounds. (18 hours)

**UNIT II ORGANOMETALLIC CHEMISTRY –II**

Oxidative addition and reductive elimination – insertion of alkenes and  $\beta$ -hydrogen elimination-Catalytic reactions- hydrogenation of olefins – Wilkinson's catalyst – hydroformylation – oxidation of olefins – Wacker process – Olefin metathesis -Ziegler Natta catalyst – ethylene polymerization - cyclo oligomerisation of acetylene , butadiene- Reppe's catalyst . Mansanto's acetic acid synthesis-Fischer-Tropsch's synthesis of Synthetic gasoline.

(18 hours)

**Unit III****Inorganic Photochemistry**

Selection rules-electronic transitions in metal complexes-Radiation relaxation rates-Metal-centered and charge transfer transitions-emission spectra-photo physical properties- Intermolecular energy transfer-collision energy transfer-Photochemical Unimolecular reactions-charge transfer photochemistry of cobalt(III)-am(m)ine complexes- Mechanism of CTM photoreactions of Co(III) complexes-Dioxygencomplexes-polydentate chelates- Photochemistry of Cr(III) complexes-Cr(III)hexam(m)ines-Adamson's rules-redox potentials- electron and energy transfer reactions- photochemistry of ruthenium-polypyridine complexes.

(18hours)

**UNIT IV ESR Spectroscopy**

Principles – presentation of a spectrum – hyperfine coupling constant- hyperfine splitting in radicals containing a single set of equivalent protons– evaluation of g tensor – Isotropy, Anisotropy in g value - factors affecting the magnitude of g – values – zero field splitting – Kramer's degeneracy – ESR of  $d^3$  octahedral complexes — application of ESR in the study of transition metal complexes –  $VO^{2+}$ ,  $Fe^{3+}$ ,  $Co^{2+}$ ,  $Mn^{2+}$ ,  $Ni^{2+}$  and bisalicylaldimine copper (II) – Jahn Teller distortion studies in Cu (II) complexes.

(18 hours)

**UNIT V NMR AND NQR SPECTROSCOPY:****a) NMR Spectroscopy:**

Multinuclear NMR-  $^{31}P$ ,  $^{19}F$  and  $^{15}N$  NMR – introduction application in structural problem -  $ClF_3$ ,  $SF_4$ ,  $PF_5$ ,  $BrF_5$ ,  $P_4S_3$ ,  $PF_3(NH_2)_2$  - evaluation of rate constants –NMR of fluxional molecules –NMR of paramagnetic molecules- contact shifts and shift reagents.

**b) NQR Spectroscopy:**

Introduction – effect of magnetic field on the spectra – relation between electric field gradient and structure – applications of NQR.

**TEXT BOOKS**

1. Gopalan, R. & Ramalingam, V. (2003). *Concise Coordination Chemistry*. New Delhi: Vikas Publishing House Pvt.Ltd., 1<sup>st</sup> Edition.
2. Drago, R.S. (1977). *Physical Methods in Chemistry*. London: Saunders Golden Suburst Series, W.B.Saunders Company, 1<sup>st</sup> Edition.
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4. Soni, P.L. & Pandna Soni. (2016). *Coordination Chemistry*. New Delhi: Ane Books Pvt.Ltd., 1<sup>st</sup> Edition.
5. Meissler G.L. and Tarr T.A., (2004) *Inorganic Chemistry*, Pearson Academy, New Delhi, 3<sup>rd</sup> Edition.

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	PSO 1.a	PSO 1.b	PSO2	PSO3 .a	PSO3 .b	PSO 4	PSO 5	PSO 6	PSO 7	PSO 8
CO 1	H	H	M	H	H	M	H	H	M	M
CO 2	H	H	M	H	H	M	H	H	M	M
CO 3	H	H	L	H	H	M	H	H	L	M
CO 4	H	H	L	H	H	M	H	H	L	M
CO 5	H	H	M	H	H	M	H	H	M	M

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VIRUDHUNAGAR - 626 001

### M.Sc. CHEMISTRY

(For those who join in the Academic Year 2020-2021)

Semester III	<b>ELECTROCHEMISTRY AND MOLECULAR SPECTROSCOPY</b>	Hours/Week: 6	
Core Course – 9		Credits: 5	
Course Code 20PCHC33		Internal 40	External 60

#### COURSE OUTCOMES

On completion of the course, the students will be able to

- CO1: summarise the fundamental concepts and theories of electrochemistry and molecular microwave, vibrational and electronic spectroscopy. [K2]
- CO2: make use of the applications of electrochemistry and molecular spectroscopy. [K3]
- CO3: outline the concepts of electrolytic conductance, electrokinetic phenomena and spectroscopic techniques such as electronic and microwave. [K3]
- CO4: analyze the physical approach of Debye-Huckel theory and microwave, IR & Raman spectra. [K4]
- CO5: evaluate the theory and applications of Butler-Volmer and Tafel equations and ESR, NMR and NQR spectroscopic techniques. [K5]

#### UNIT I

##### Electrochemistry I

Ions in solutions – electrolytic conductance - Dispersion of conductance at high frequencies (Debye – Falkenhagen effect). Conductance with high potential gradients (Wien effect) - Activity and activity coefficient, activities of electrolytes and mean ion activity coefficient - relaxation and electrophoretic effects - Debye – Huckel theory of strong electrolytes – Debye – Huckel – Onsager equation – verification and limitation – Detailed treatment of ion – solvent interactions (ion solvation), solvation number - Energy conduction: Ion – ion interactions (ion – association) - Bjerrum's theory of ion – association. (18 Hours)

## UNIT II

### Electrochemistry – II

Electrokinetic phenomena: Electrical double layer - Helmholtz Perrin, Gouy- Chapman and Stern models.- Electroosmosis, Streaming potential.

Polarisation and over voltage - Energy barrier at electrode surface: overpotential, Butler – Volmer equation – derivation - Tafel equation- Electrochemical energy systems – Corrosion and passivation of metals – Pourbaix diagram – Evans diagram.

(18 Hours)

## UNIT III

### Molecular Spectroscopy – I

Introduction to electromagnetic radiation and its interaction with atoms and molecules - Quantization of energy- regions and representation of spectra- Einstein absorption and emission coefficient -Fourier transform spectroscopy.

Microwave Spectroscopy Rotational spectra of diatomic molecules - Rigid rotators: rotational energy levels, intensity of spectral lines, selection rules, effect of isotopic substitution- Rotational spectra of linear and symmetric top polyatomic molecules- Microwave spectrometer-Information derived from rotational spectra. (18 Hours)

## UNIT IV

### Molecular Spectroscopy – II

Molecular Vibrational Spectroscopy -Harmonic and anharmonic vibrations: wave functions, selection rules, Morse oscillator- Diatomic vibrating rotator: Born-oppenheimer approximation, vibration-rotation spectra, selection rules, P, Q, R branches- Vibrational motion in Polyatomic molecules: symmetry and fundamental vibrations, normal modes, overtones, combination, difference bands-Fermi resonance-concept of group frequencies.

Raman spectroscopy: Theories of Raman scattering-Rotational Raman spectra-Vibrational Raman spectra-Mutual exclusion principle- Rotation-vibration Raman spectra of diatomic molecules - Molecular structure determination from Raman and Infra-red spectroscopy.

(18 Hours)

## UNIT V

### Molecular Spectroscopy – III

Electronic spectroscopy of diatomic and polyatomic molecules- Intensity of vibrational electronic spectra- Franck- Condon principle-rotation fine structure of electronic vibrational spectra- the Fortrat parabola-Dissociation and predissociation spectra –Induced emission.

Spin Resonance Spectroscopy; the nature of spinning particles, interaction between spin and magnetic field, Larmor precession - Nuclear Magnetic Resonance Spectroscopy: The chemical shift-The coupling constant-Coupling between several nuclei- Bloch equations - NMR instrumentation – ENDOR – Overhauser effect.

Electron spin resonance spectroscopy: The theory of E.S.R- The position of E.S.R. absorption-The g factor- The fine and hyperfine structures of E.S.R. absorption-Applications of E.S.R. spectroscopy. (18 Hours)

### TEXT BOOKS

1. Puri, B.R. Sharma, L.R. Pathania, M.S. (2003). *Principles of Physical Chemistry*. New Delhi: Vishal Publishing Co, 1<sup>st</sup> Edition.
2. Gurdeep Raj,(2001).*Advanced Physical Chemistry*. Chennai: Goel Publishing Co., 25<sup>th</sup> Edition.
3. Aruldas, G.(2001).*Molecular Structure and Spectroscopy*. New Delhi: Prentice – Hall of India Pvt. Ltd., 1<sup>st</sup> Edition.
4. Drago, R.S.(1977). *Physical Methods in Chemistry*. London: W.B. Saunders Co., 1<sup>st</sup> Edition.
5. Bajpai, D.N. (2012). *Advanced Physical Chemistry*. New Delhi: S.Chand & Company Ltd., 4<sup>th</sup> Edition
6. Banwell, C.N. & McCash, E.M. (2000). *Molecular Spectroscopy*. New York:Tata McGraw Hill,4<sup>th</sup> Edition.
7. Chang, R. (1976). *Basic Principles of Spectroscopy*. London: McGraw Hill, 1<sup>st</sup> Edition.

### REFERENCES BOOKS

1. Barrow, G.M.(2000). *Introduction to Molecular Spectroscopy* New York: McGraw Hill, 1<sup>st</sup> Edition.
2. Straughan, B.F.& Walker, S.(1976). *Spectroscopy*. Vol.1,2,3, London: Chapman & Hall, 1<sup>st</sup> Edition.
3. Atkins, P.W. (2001).*Physical Chemistry*.Tokyo: Oxford University Press, 6<sup>th</sup> Edition.

4. Bockris, O.M. Reddy, K.N. and Gamboa – Aldeco,( 2000) *Modern Electrochemistry* 2A. New York : Kluwer Academic/ Plenum Publishers, , 2<sup>nd</sup> Edition.
5. Castellan, G.W. (2011) *Physical Chemistry*. New Delhi: Narosa Publishing House, , 2<sup>nd</sup> Edition.
6. Glasstone, S.(2006) *An Introduction to Electrochemistry*. New Delhi: East-West Press Pvt. Ltd., 1<sup>st</sup> Edition.

Course Code 20PCHC33	PO1		PO2	PO3		PO4	PO5	PO6	PO7	PO8
	PSO 1.a	PSO 1.b	PSO 2	PSO 3.a	PSO 3.b	PSO 4	PSO 5	PSO 6	PSO 7	PSO 8
CO1	H	H	H	H	H	H	M	M	M	M
CO2	H	H	H	H	H	H	M	M	M	M
CO3	H	H	H	H	H	H	M	M	M	H
CO4	H	H	H	H	H	H	M	M	M	H
CO5	H	H	H	H	H	H	M	M	M	H

Dr. J. Kavitha  
Head of the Department

Dr.J.Kavitha  
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Course Designers



## V.V.VANNIAPERUMAL COLLEGE FOR WOMEN

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**VIRUDHUNAGAR - 626 001**

### M.Sc. CHEMISTRY

(2023-2024 onwards)

Semester III	<b>ELECTROCHEMISTRY AND MOLECULAR SPECTROSCOPY</b>	Hours/Week: 6	
Core Course – 9		Credits: 5	
Course Code 20PCHC33N		Internal 40	External 60

### COURSE OUTCOMES

On completion of the course, the students will be able to

- CO1: Summarise the fundamental concepts and theories of electrochemistry and molecular microwave, vibrational and electronic spectroscopy. [K2]
- CO2: Make use of the applications of electrochemistry and molecular spectroscopy. [K3]
- CO3: Outline the concepts of electrolytic conductance, electrokinetic phenomena and spectroscopic techniques such as electronic and microwave. [K3]
- CO4: analyze the physical approach of Debye-Huckel theory and microwave, IR & Raman spectra. [K4]
- CO5: evaluate the theory and applications of Butler-Volmer and Tafel equations and molecular spectroscopic techniques. [K5]

### UNIT I

#### Electrochemistry I

Theory of strong electrolytes – Interionic attraction theory – Debye-Huckel theory of strong electrolytes - Debye-Huckel model of ionic atmosphere–Debye-Huckel Onsager equation-derivation, verification and modifications- Debye – Falkenhagen effect and Wien effect; Electrical double layers – formation – Structure of electrified interfaces – Stern model. Debye-Huckel limiting law- extension- Huckel-Bronsted equation - Determination of activity coefficients using Bronsted equation – Applications of conductivity measurements; Nernst equation and its significance – reversible and irreversible cells - electrodes – SHE – Calomel – Glass electrode – Platinum electrode – Glassy carbon electrode – ion selective electrode and measurement of pH. (18 Hours)

**UNIT II****Unit-II: Electrochemistry-II**

Over voltage – theories of over voltage- applications of over voltage-hydrogen and oxygen overvoltage; Butler-Volmer equation- Tafel equation; Corrosion- principles of electrochemical corrosion – dry and wet corrosion and its mechanism – Pilling-Bedworth rule. Types of corrosion- galvanic, aeration, stress, pitting corrosion and passivity – factor influencing corrosion – corrosion control- cathodic production - corrosion inhibitors.

Principles of Polarography - Cyclic Voltametry –quasi – reversible – irreversible voltamogram; electrochemical energy conversions-Nickel Cadmium, lead acid battery; Fuel cells – H<sub>2</sub> - O<sub>2</sub> Fuel cell – methyl alcohol fuel cell. (18 Hours)

**UNIT III****Molecular Spectroscopy – I: Rotational & Vibrational Spectroscopy**

Introduction to electromagnetic radiation and its interaction with atoms and molecules - Quantization of energy- regions and representation of spectra.

Rotational Spectroscopy: Rotational spectra of diatomic molecules, effect of isotopic substitution- Rotational spectra of linear and symmetric top polyatomic molecules- Microwave spectrometer-Information derived from rotational spectra.

Vibrational spectra of a diatomic molecule- Vibrational spectra of polyatomic molecule- Fermi resonance. Rotation-vibration spectra of polyatomic molecule: linear molecule, symmetric top molecule. Over tones, combination frequencies and group frequencies. IR spectrophotometer-Instrumentation. (18 Hours)

**UNIT IV Molecular Spectroscopy – II: Raman and Photo Electron Spectroscopy**

Raman spectroscopy: Theory of Raman scattering: Classical and Quantum theory. Rotational Raman Spectra: linear molecule, symmetric top molecule, spherical top molecule. Vibrational Raman spectra of diatomic molecule. Mutual exclusion principle.

**Photo Electron Spectroscopy:** Principle, Instrumentation – XPS, UPS, ESCA

(18 Hours)

**UNIT V****Molecular Spectroscopy – III: Electronic and NMR spectroscopy**

Electronic spectroscopy: Vibrational coarse Intensity of vibrational electronic spectra- Franck- Condon principle-Rotation fine structure of electronic vibrational spectra- the Fortrat parabola-Dissociation and predissociation spectra .

NMR Spectroscopy: Theory – Relaxation processes - spin-spin relaxation and spin-lattice relaxation. Bloch equations - NMR instrumentation – Nuclear Overhauser effect.

(18 Hours)

**UNIT V****Molecular Spectroscopy – III: Electronic and NMR spectroscopy**

Electronic spectroscopy: Vibrational coarse Intensity of vibrational electronic spectra- Franck- Condon principle-Rotation fine structure of electronic vibrational spectra- the Fortrat parabola-Dissociation and predissociation spectra .

NMR Spectroscopy: Theory – Relaxation processes - spin-spin relaxation and spin-lattice relaxation. Bloch equations - NMR instrumentation – Nuclear Overhauser effect.

(18 Hours)

**TEXT BOOKS**

1. Puri, B.R. Sharma, L.R. Pathania, M.S. (2003). *Principles of Physical Chemistry*. New Delhi: Vishal Publishing Co, 1<sup>st</sup> Edition.
2. Gurdeep Raj,(2001).*Advanced Physical Chemistry*. Chennai: Goel Publishing Co., 25<sup>th</sup> Edition.
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1. Barrow, G.M.(2000). *Introduction to Molecular Spectroscopy* New York: McGraw Hill, 1<sup>st</sup> Edition.
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3. Atkins, P.W. (2001).*Physical Chemistry*.Tokyo: Oxford University Press, 6<sup>th</sup> Edition.
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5. Castellan, G.W. (2011) *Physical Chemistry*. New Delhi: Narosa Publishing House, , 2<sup>nd</sup> Edition.

6. Glasstone, S.(2006) *An Introduction to Electrochemistry*. New Delhi: East-West Press Pvt. Ltd., 1<sup>st</sup> Edition.

Course Code 20PCHC33N	PO1		PO2	PO3		PO4	PO5	PO6	PO7	PO8
	PSO 1.a	PSO 1.b	PSO 2	PSO 3.a	PSO 3.b	PSO 4	PSO 5	PSO 6	PSO 7	PSO 8
CO 1	H	H	H	H	H	H	M	M	M	M
CO 2	H	H	H	H	H	H	M	M	M	M
CO 3	H	H	H	H	H	H	M	M	M	H
CO 4	H	H	H	H	H	H	M	M	M	H
CO 5	H	H	H	H	H	H	M	M	M	H

Dr. J. Kavitha  
Head of the Department

Dr.J.Kavitha  
Dr.N.Ramiladevi  
Course Designers



**M.Sc. CHEMISTRY**

**(For those who join in the Academic Year 2020-2021)**

Semester III	<b>PHYSICAL CHEMISTRY EXPERIMENTS</b>	Hours/Week: 6	
Core Practical -3		Credits: 3	
Course Code <b>20PCHC31P</b>		Internal 40	External 60

**COURSE OUTCOMES**

On completion of the course, the students will be able to

- CO1: apply standard procedure to carryout the various types of conductometric titrations. [K3]
- CO2: apply standard procedure to carryout the various types of potentiometric titrations. [K3]
- CO3: develop analytical skill to perform adsorption experiments. [K3]
- CO4: examine the metal ions such as Cu<sup>2+</sup>, Fe<sup>2+</sup> and Ni<sup>2+</sup> ions by spectrophotometric techniques. and compare their strengths with the standard solution. [K4]
- CO5: interpret the spectral results obtained of the unknown compounds by using pHmeter, UV-Vis and IR specrophotometric techniques. [K5]

**I. Conductometric Experiments**

i. Double displacement & acid-base titrations



ii. Estimation of BaCl<sub>2</sub> by conductometric precipitation titration

iii. Determination of solubility product of sparingly soluble salts, and dissociation constant of weak acids.

**II. Adsorption Experiments**

Adsorption of oxalic acid / Acetic acid on charcoal

**III. Kinetic Experiments**

Perdisulphate and iodide ion reaction: Study of primary salt effect and determination of the concentration of given KNO<sub>3</sub>

**IV. Potentiometric methods**

- i. Precipitation titration:  $\text{Ag}^+$  Vs halide mixture
- ii. Redox titrations:

Ceric ammonium sulphate/ potassium dichromate Vs ferrous ion

- iii. Determination of pH of buffer solution & solubility product of sparingly soluble salts.

**V. Titrations using pH meter**

Determination of first, second and third dissociation constants of phosphoric acid.

**VI. Experiments based on UV - Visible and IR spectrometer****VIII. Determination of Cu, Ni and Fe ions by Spectro Photometric method**

Course Code 20PCHC31P	PO1		PO2	PO3		PO4	PO5	PO6	PO7	PO8
	PSO 1.a	PSO 1.b	PSO 2	PSO 3.a	PSO 3.b	PSO 4	PSO 5	PSO 6	PSO 7	PSO 8
CO1	H	H	H	H	H	H	M	M	M	M
CO2	H	H	H	H	H	H	M	M	M	M
CO3	H	H	H	H	H	H	M	M	M	M
CO4	H	H	H	H	H	H	M	M	M	M
CO5	H	H	H	H	H	H	M	M	M	M

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### M.Sc. CHEMISTRY

(2023-2024 onwards)

Semester III	CHEMISTRY FOR COMPETITIVE EXAMINATION	Hours/Week: 6	
NMEC		Credits: 4	
Course Code <b>20PCHN31N</b>		Internal 40	External 60

### COURSE OUTCOMES

On completion of the course, the students will be able to

- CO1: know the fundamentals of chemistry. [K1]
- CO2: understand the basics of chemistry like elements, symbols, important laws and chemical process in chemistry, concepts of acid and bases, water and their types, environmental chemistry, nuclear chemistry, and chemistry in service of man. [K2]
- CO3: identify the types of chemical reactions, water, solutions, chemical processes, environmental pollutions, nature of metals, chemical formulae, symbol of atoms, polymers, cement, lubricants, soaps, fuels, corrosion, food adulterants, antibiotics, vitamins, and concepts of acids and bases. [K3]
- CO4: analyze the rudiment in chemistry, environmental pollutions, and chemistry in service of man. [K4]
- CO5: interpret important basic terms, concepts, laws, chemical processes, environmental chemistry, and chemistry in service of man. [K5]

### UNIT I CONCEPTS IN CHEMISTRY- I:

Atomic theory: Dalton's and Bohr's theory. Molecules: atomic and molecular mass, empirical and molecular formula. Definition of ore, mineral, alloy with examples. Types of chemical reactions: exothermic and endothermic, oxidation and reduction, addition, substitution and elimination reactions – ideal and real gas : definition. Some Basic laws in chemistry: Boyle's law, Charle's law, Grahams law of diffusion, Beer's law, Henry's law, Faraday's law, Law of conservation of mass, Hess's law,). (18 Hours)

**UNIT II CONCEPTS IN CHEMISTRY- II: (Only elementary idea can be given)**

Concepts of Acids and Bases (Arrhenius, Bronsted and Lewis) – pH concept, Buffer solution: definition and types of buffer– Water – Hard and soft water – hardness of water and types- determination of hardness of water by ion exchange process. Solutions and their types: True, Colloidal and suspension – Applications of colloids – Nuclear Chemistry – definitions of isotones, isobars, isotopes - Types of radiation: alpha, beta, gamma radiation.

(18 Hours)

**UNIT III ENVIRONMENTAL CHEMISTRY:**

Pollution and types of pollutions – Air, Water, land, Radioactive pollution.

Air pollution- Causes and control measures. Green house effect, Ozone depletion and Acid rain.

Water Pollution - Causes – effect of water pollution on groundwater and ocean-BOD, COD - control measures

Soil Pollution: Sources: common soil pollutants, effects of soil pollution-soil erosion, remedial measures.(18 Hours)

Radioactive pollution: sources, harmful effects of radioactive pollutants, nuclear waste and its disposal methods, control measures of radioactive pollution. (18 Hours)

**UNIT IV CHEMISTRY IN DAY TO DAY LIFE: (Only elementary idea can be given)**

Plastics – Types with examples – Polymer: definition, Types of polymer - natural and synthetic polymers with example. Glass – Annealing of glass – Cement – Constituents and setting of cement – Rubber – Types with examples and vulcanization of rubber- Corrosion of metal – prevention – Lubricants -definition and classification. Fuel – Types with suitable examples - calorific value – Composition of LPG and Rocket fuel.

(18 Hours)

**UNIT V CHEMISTRY IN SERVICE OF MANKIND –II: (Only elementary idea can be given)**

Food adulterants – common food adulterants and their harmful effects and tests to identify them–Sources and deficiency of Vitamins A, B6, B12, C, D, E and K (structural elucidation not required) –Structure and therapeutic uses of antibiotics – penicillin, chloroamphenicol, streptomycin and tetracycline. (18 Hours)

**TEXT BOOKS**

1. Puri, B.R. Sharma, L.R. Pathania, M.S. (2003). *Principles of Physical Chemistry*. New Delhi: Vishal Publishing Co, 1<sup>st</sup> Edition.
2. Puri, B.R. Sharma, L.R. & Kalia, K.C. (2008). *Principles of Inorganic Chemistry*, New Delhi: Milestone Publishers, 2<sup>nd</sup> Edition.
3. Sharma, B. K.(2008). *Industrial Chemistry*. Meerut:GOEL Publishing House, 1<sup>st</sup> Edition.
4. Jayashree Ghosh, (2013). *Fundamental Concepts of Applied Chemistry*, New Delhi: S.Chand & Company Ltd.,1<sup>st</sup> Edition.
- 5 BagavathiSundari, K.(2008). *Applied Chemistry*. Chennai: MJP Publishers, 1<sup>st</sup> Edition.
6. Tyagi, O.D.and Mehra, M.(2002). *A Text book of Environmental Chemistry*. New Delhi: Anmol Publication, 1<sup>st</sup> Edition.
7. General Studies Manual,( 2013) The TMH Publishers.
8. Ramani,V.(2014).*Food Chemistry*. Chennai: MJP Publishers, 1<sup>st</sup> Edition.

**REFERENCE BOOKS**

1. Jain, P.C. & Monika Jain, (2013). *Engineering Chemistry*.New Delhi: DhanpatRai Publishing Company Pvt.Ltd., 1<sup>st</sup> Edition.
2. Jayashree Ghosh. ( 2014).*A Text Book of Pharmaceutical Chemistry*. New Delhi: S.Chand & Company Ltd, 3<sup>rd</sup> Edition.
3. Dara,S.S. (2004). *A Text book of Environmental Chemistry and Pollution Control*. New Delhi: S.Chand & Company Ltd., 7<sup>th</sup> Edition.

Course Code 20PCHN31N	PO1		PO2	PO3		PO4	PO5	PO6	PO7	PO8
	PSO 1.a	PSO 1.b	PSO 2	PSO 3.a	PSO 3.b	PSO 4	PSO 5	PSO 6	PSO 7	PSO 8
CO1	H	H	H	H	H	H	M	M	M	M
CO2	H	H	H	H	H	H	M	M	M	M
CO3	H	H	H	H	H	H	M	M	M	M
CO4	H	H	H	H	H	H	M	M	M	M
CO5	H	H	H	H	H	H	M	M	M	M

Dr. J. Kavitha  
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Dr.M.Vairalakshmi  
Course Designers



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VIRUDHUNAGAR - 626 001

M.Sc Chemistry  
(2021 -22 onwards)

Semester III	<b>PRACTICE FOR CSIR NET – GENERAL PAPER</b>	<b>Hours/Week:1</b>	
Course Code		<b>Credits: 1</b>	
20PGOL32		<b>Internal 100</b>	<b>External -</b>

### COURSE OUTCOMES

On completion of the course, the students will be able to

- CO1 : explain various concepts related to numbers, quantitative comparison, monetary problems and logical reasoning. [K2]
- CO2 : apply the analytical skills and logical reasoning in solving problems related to competitive examinations. [K3]
- CO3 : solve typical problems, geometrical type problems, daily life problems in an effective manner. [K3]
- CO4 : analyze the techniques used in solving complicated real life problems.[K4]
- CO5 : interpret the data using logical reasoning and observational ability.[K5]

### UNIT I

**Typical Problems-** Series formation

**Numerical Ability-** Numbers

### UNIT II

**Geometrical Type Problems**

Mensuration and quantitative comparison

### UNIT III

**Typical Problems-** Moving locomotive problem

**Numerical Ability-** Distance and Directions

**UNIT IV****Daily Life Problems**

Finding the X – Average - Monetary problems

**UNIT V****Logical Reasoning**

Data interpretation – Observational ability – Logical puzzles

**BOOKS FOR STUDY:**

Christy Varghese (2016)., *CSR – NET, General aptitude –A new outlook*, Lilly publishing house, Changanacherry, Kerala

**REFERENCE BOOKS**

1. Pradip Kumar Ray, General Aptitude Theory ,CSIR NET, Previous question and answer with explanation and hint to solve, Notion Press, India
2. Ram Mohan Pandey (2021)., *CSIR-UGC-NET General Aptitude Theory and Practice*, Pathfinder Publication, a unit of Pathfinder Academy Pvt. Ltd., India.

Unit	Chapter	Section/Page Number
1	4	142-162
	5	163-192
2	12	272-294
3	3	132-141
	7	206-220
4	8	221-230
	9	231-239
	10	240-249
5	13	295-309
	14	310-323
	15	324-332

Course code 20PGOL32	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8
CO1	H	H	M	M	-	M	-	-
CO2	H	H	H	H	-	M	-	-
CO3	H	H	H	H	-	H	-	-
CO4	H	M	H	H	-	H	-	-
CO5	H	M	H	H	-	H	-	-

Dr.A.Uma Devi  
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Dr.A.Uma Devi  
Tmty.T.Anitha  
Course Designer



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**M.Sc. CHEMISTRY**

(For those who join in the Academic Year 2020-2021)

Semester IV	<b>HETEROCYCLES , NATURAL PRODUCTS AND ANALYTICAL TECHNIQUES</b>	Hours/Week: 6	
Core Course-10		Credits: 5	
Course Code 20PCHC41		Internal 40	External 60

**COURSE OUTCOMES**

On completion of the course, students will be able to

- CO1: comprehend the structural and synthetic aspects of biomolecules, heterocycles and natural products and describe the analytical techniques. [K2]
- CO2: predict the ring size in carbohydrates, elucidate the structure of natural products, sketch the preparation of heterocycles and apply the Octant rule in determining the configuration and conformation of simple monocyclic and bicyclic ketones. [K3]
- CO3: interpret the structure of RNA and DNA, demonstrate the synthesis of biomolecules, relate the structure and reactivity of heterocycles, natural products and practice chromatographic techniques. [K3]
- CO4: analyze the synthetic routes to peptides, heterocycles, and natural products and relate CD and ORD curves. [K4]
- CO5: categorize the significance of biomolecules, heterocycles and natural products in day to-day life and plan the suitable chromatographic technique for their project. [K5]

**UNIT I Proteins, Nucleic acids and Carbohydrates :**

Classification of proteins – peptides – structure of peptides – chemistry of glutathione and oxytocin – structure of proteins

Nucleic acid- chemistry of nucleic acid, nucleosides and nucleotides-structure of RNA and DNA and their biological importance.

Pyranose and furanose forms of aldohexoses and ketohexoses – methods used for determination of ring size – conformations of aldohexopyranoses – structure and synthesis of lactose and sucrose. A brief study of starch and cellulose. (18 Hours)

**UNIT II Heterocycles:**

Structure, synthesis and their reaction of the following systems- a) One heteroatom – furan, thiophene, pyridine, isoquinoline b) Benzo fused heterocycles-indole, quinoline c) Two heteroatoms – pyrazole, imidazole, pyrimidine, pyrazine . (18 Hours)

**UNIT III Alkaloids:**

General methods of structural determination- Hofmann, Emde and Von Braun degradations. Structure and synthesis of quinine, papaverine, atropine, narcotine, morphine, reserpine and lysergic acid. (18 Hours)

**UNIT IV Terpenoids and Steroids:****Terpenoids:**

Classification of terpenoids – structural elucidation and synthesis of  $\alpha$  – pinene, camphor, zingiberene, cadinene, abietic acid.

**Steroids:**

Classification – conformational aspects of A/B *cis* and A/B *trans* steroids – complete chemistry and stereochemistry of cholesterol – male sex hormone- testosterone – female sex hormones – oestrone and progesterone- biosynthesis of sterols, bile acids. (18 Hours)

**UNIT V Chiro optical and Analytical techniques:**

ORD and CD – Principle – Cotton effect – types of ORD curves –  $\alpha$  -haloketone rule – Octant rule – applications to determine the configuration and conformation of simple monocyclic and bicyclic ketones – comparison of ORD and CD.

**Chromatographic techniques:** Principle and applications of Column chromatography, GLC, HPLC, GC-MS and LC-MS. (18 Hours)

**TEXT BOOKS**

1. Chatwal, G.R. (2018). *Organic Chemistry of Natural Products. Vol.I&II*, Mumbai: Himalaya Publishing House, 5<sup>th</sup> Edition.
2. Agarwal, O.P. (2017). *Chemistry of Organic Natural Products. Vol.I*, Meerut: Goel Publishing House, 47<sup>th</sup> Edition.
3. Agarwal, O.P. (2018), *Chemistry of Organic Natural Products. Vol.II*, Meerut: Goel Publishing House, 46<sup>th</sup> Edition.
4. Finar, I.L. (2003). *Organic Chemistry. Vol.II.*, Singapore: Pearson Education, 5<sup>th</sup> Edition.

5. Ireland, R.E. (1975). *Organic Synthesis*. New York: Prentice-Hall of India Pvt. Ltd., 1<sup>st</sup> Edition
6. Jagdamba Singh, Yadav L.D.S. (2014). *Organic Synthesis*. Meerut: PragatiPrakashan, 1<sup>st</sup> Edition.

### REFERENCE BOOKS

1. Klyne, W (1965). *The Chemistry of Steroids*. New York: Methuen & Co., 1<sup>st</sup> Edition.
2. Crabbe, P. (1972). *ORD and CD in Chemistry and Biochemistry*. Cambridge: Academic Press. 1<sup>st</sup> Edition.
3. Braithwaite, A. & Smith, F.J. (1985). *Chromatographic Methods*. London: Chapman and Hall, 4<sup>th</sup> Edition.

Course Code 20PCHC41	PO1		PO2	PO3		PO4	PO5	PO6	PO7	PO8
	PSO 1.a	PSO 1.b	PSO 2	PSO 3.a	PSO 3.b	PSO 4	PSO 5	PSO 6	PSO 7	PSO 8
CO1	H	M	H	M	M	H	M	M	M	L
CO2	H	H	M	M	M	H	M	M	L	L
CO3	H	H	M	M	M	M	M	M	H	H
CO4	H	H	M	M	L	H	M	M	L	L
CO5	H	H	H	H	M	H	H	H	H	H

Dr. J. Kavitha  
Head of the Department

Mrs.R.Nagasathya  
Mrs.A.Prasanna  
Course Designers



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VIRUDHUNAGAR - 626 001

### M.Sc. CHEMISTRY (2022-2023 onwards)

Semester IV	<b>Heterocycles, natural products and analytical techniques</b>	Hours/Week: 6	
Core Course-10		Credits: 5	
Course Code 20PCHC41N		Internal 40	External 60

#### COURSE OUTCOMES

On completion of the course, students will be able to

- CO1: comprehend the structural and synthetic aspects of biomolecules, heterocycles and natural products and describe the analytical techniques. [K2]
- CO2: predict the ring size in carbohydrates, elucidate the structure of natural products, sketch the preparation of heterocycles and apply the Octant rule in determining the configuration and conformation of simple monocyclic and bicyclic ketones. [K3]
- CO3: interpret the structure of RNA and DNA, demonstrate the synthesis of biomolecules, relate the structure and reactivity of heterocycles, natural products and practice chromatographic techniques. [K3]
- CO4: analyze the synthetic routes to peptides, heterocycles, and natural products and relate CD and ORD curves. [K4]
- CO5: categorize the significance of biomolecules, heterocycles and natural products in day-to-day life and plan the suitable chromatographic technique for their project. [K5]

#### UNIT I Heterocycles:

Nomenclature of heterocycles having not more than two hetero atoms-structures, and reactions of Oxazole, Coumarin, Flavone and Flavanol (3-hydroxyflavone), Anthocyanins (Quercetin, cyanin, cyanidin chloride)- Pyrimidines (uracil) and Purines (synthesis of Caffeine, Theobromine and theophylline. (18 Hours)

#### UNIT II Proteins, Nucleic acids and Carbohydrates:

Classification of proteins –peptides-structure and synthesis of peptides-Chemistry of glutathione and oxytocin-an elementary treatment of enzymes, coenzyme and nucleic acids-

biosynthesis of amino acids-RNA and protein synthesis-Genetic code-DNA and determining the basic sequence of DNA.

Pyranose and furanose forms of aldohexoses and keto hexoses-methods used for determination of ring size- structure and synthesis of lactose, cellobiose. A brief study of starch and cellulose. (18 Hours)

### UNIT III Alkaloids and Terpenoids:

General methods of structural determination of alkaloids- Hofmann, Emde and Von Braun degradations. Structure and synthesis of quinine, papaverine, atropine, narcotine, morphine. Biogenesis of Alkaloids.

Classification of terpenoids – structural elucidation and synthesis of  $\alpha$  – pinene, cadinene, abietic acid. Biogenesis of Terpenoids. (18 Hours)

### UNIT IV Steroids and Chiro optical techniques:

Classification –conformational aspects of A/B *cis* and A/B *Trans* steroids – complete chemistry and stereochemistry of cholesterol – male sex hormone- testosterone – female sex hormones – oestrone and progesterone.

ORD and CD – Principle – Cotton effect – types of cotton effect curves –  $\alpha$  -haloketone rule – Octant rule – applications to determine the configuration and conformation of simple monocyclic and bicyclic ketones – application of CD- advantages and Limitation of ORD and CD. Application of ORD measurements to steroid ketones. (18 Hours)

### UNIT V Flavonoids and Isoflavonoids:

**Flavonoids:** Introduction, isolation and separation techniques of flavonoids, general method for determination of the structure of flavone – Rutin and Quercetin

**Isoflavonoids:** Occurrence and biosynthesis pathway of isoflavones. (18 hours)

### TEXT BOOKS

1. Chatwal, G.R. (2018). *Organic Chemistry of Natural Products. Vol.I&II*, Mumbai: Himalaya Publishing House, 5<sup>th</sup> Edition.
2. Agarwal, O.P. (2017). *Chemistry of Organic Natural Products. Vol.I*, Meerut: Goel Publishing House, 47<sup>th</sup> Edition.
3. Agarwal.O.P. (2018), *Chemistry of Organic Natural Products. Vol.II*, Meerut:Goel Publishing House, 46<sup>th</sup> Edition.
4. Finar, I.L. (2003).*Organic Chemistry. Vol.II.*,Singapore:Pearson Education,5<sup>th</sup> Edition.

5. Ireland, R.E. (1975). *Organic Synthesis*. New York: Prentice-Hall of India Pvt. Ltd., 1<sup>st</sup> Edition
6. Jagdamba Singh, Yadav L.D.S. (2014). *Organic Synthesis*. Meerut: PragatiPrakashan, 1<sup>st</sup> Edition.
7. Gurdeep R. Chatwal (2016), *Organic Chemistry of Natural Products*, Himalaya Publishing House, 4<sup>th</sup> Edition.

#### REFERENCE BOOKS

1. Klyne, W. (1965). *The Chemistry of Steroids*. New York: Methuen & Co., 1<sup>st</sup> Edition.
2. Crabbe, P. (1972). *ORD and CD in Chemistry and Biochemistry*. Cambridge: Academic Press. 1<sup>st</sup> Edition.

Course Code 20PCHC41N	PO1		PO2	PO3		PO4	PO5	PO6	PO7	PO8
	PSO 1.a	PSO 1..b	PSO 2	PSO 3.a	PSO 3..b	PSO 4	PSO 5	PSO 6	PSO 7	PSO 8
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CO 2	H	H	M	M	M	H	M	M	L	L
CO 3	H	H	M	M	M	M	M	M	H	H
CO 4	H	H	M	M	L	H	M	M	L	L
CO 5	H	H	H	H	M	H	H	H	H	H

Dr. J. Kavitha

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**VIRUDHUNAGAR - 626 001**

**M.Sc. CHEMISTRY**

**(For those who join in the Academic Year 2020-2021)**

Semester IV	<b>CHEMICAL KINETICS, SURFACE AND BIOPHYSICAL CHEMISTRY</b>	Hours/Week: 6	
Core Course 11		Credits: 5	
Course Code <b>20PCHC42</b>		Internal 40	External 60

### COURSE OUTCOMES

On completion of the course, the students will be able to

- CO1: extend the fundamental concepts and theories of reaction rate in kinetics, surface and biophysical chemistry. [K2]
- CO2: make use of the principle and applications of kinetics, Biophysical, surface and Supramolecular chemistry. [K3]
- CO3: develop advanced knowledge of catalysis, kinetics of complex reactions, Bioenergetics, Photo and Radiation Chemistry. [K3]
- CO4: analyze the concepts of the fast reactions, biomolecular techniques, self assembly in supramolecular chemistry, surface and radiation chemistry. [K4]
- CO5: evaluate about complex reactions, catalysis, radiation chemistry, biomolecular study and molecular recognition. [K5]

### UNIT I

#### Chemical Kinetics

Theories of reaction rates – Arrhenius theory, Hard sphere collision theory and transition state theory of reaction rates– Comparison of collision theory and activated complex theory – Theory of unimolecular reactions-Lindemann, Hinshelwood, RRKM and Slater treatment-steady state approximation- kinetic isotope effect - ARRT to reaction in solution - influence of solvent, ionic strength, and pressure on reactions in solution - Significance of volume and entropy of activation - Primary and secondary salt effect.

Kinetics of complex reactions – reversible reactions, consecutive reactions – Parallel reactions and Chain reactions - photochemical  $H_2 - Cl_2$  reaction. –Rice Herzfeld mechanism of dissociation of organic molecules viz. dissociation of ethane, decomposition of acetaldehyde –study of  $H_2- O_2$  explosive reactions - Study of fast reactions: Relaxation methods-temperature and pressure jump methods - Stopped flow technique, flash photolysis and Crossed molecular beam method. (18 Hours)

## UNIT II Surface Chemistry and Catalysis

Adsorption-Physical and chemical adsorption – adsorption isotherms – Langmuir, Freundlich and B.E.T-Temkin adsorption isotherms – measurement of surface area from BET - Adsorption on liquid surface-surface tension-Gibbs's adsorption isotherm. Mechanism of surface reactions, unimolecular and bimolecular surface reactions, Langmuir – Hinshelwood mechanism for gases only.

Catalysis- acid – base catalysis - Bronsted catalysis law –heterogeneous catalysis- Enzyme catalysis – effect of substrate concentration- Michaelis – Menton equation-effect of pH and temperature on enzyme catalysis. (18 Hours)

## UNIT III

### Photo and Radiation Chemistry

Photophysical processes of electronically excited molecules - Franck – Condon principle a quantum – mechanical treatment - Excited state dipole moment and acidity constant - Absorption and emission of radiation – decay of electronically excited states – radiative and non –radiative processes – Fluorescence and Phosphorescence – Prompt and delayed fluorescence – quenching of fluorescence – static and dynamic quenching; Stern – Volmer equation – Excimers and exciplexes - Kinetics of Photochemical reactions – Photosensitized reactions. Photovoltaic and photogalvanic cells – photoelectrochemical cells – solar cells- solar energy conversion.

Radiation Chemistry – radiolysis of water – definition of G-value – mode of reactions of hydrated electrons –  $OH$  and  $H$  – Experimental techniques of radiation chemistry – Dosimetry. (18 Hours)

**UNIT IV****Biophysical Chemistry**

Transport and storage of metals: The transport mechanism - transport of alkali and alkaline earth metals –ionophores - transport by neutral macrocycles and anionic carriers - sodium/potassium pump - transport and storage of Iron (Transferrin & Ferritin).

Bio-Energetics: Thermodynamic Considerations - standard free energy change in biochemical reactions – exergonic - endergonic reactions - hydrolysis of ATP and its synthesis from ADP.

Technique for bio-molecular study: Principle and factors affecting electro-phoretic mobility – Types of electrophoresis - zone electrophoresis–Paper electrophoresis, cellulose acetate electrophoresis, Gel electrophoresis and Capillary Electrophoresis, - Application of electrophoresis. (18 Hours)

**UNIT V****Supramolecular Chemistry**

Introduction - Molecular Recognition - Principles of molecular receptor designs- Spherical recognition (cryptates of metal cations) - Tetrahedral recognition by macro tricyclic cryptands - Recognition of ammonium ions - Recognition of neutral molecules and anionic substrates (anionic coordination) – Self assembly in supramolecular chemistry – Uses of supramolecules – Zeolites, Cyclodextrin, cryptands, calixarenes, rotaxanes, clathrates and Calixarenes. (18 Hours)

**TEXT BOOKS**

1. Puri, B.R. Sharma, L.R. & Pathania, M.S. (2003). *Principles of Physical Chemistry*. Jalandhar, Delhi: (Millennium Edn.) Vishal Publishing Co., 1<sup>st</sup> Edition.
2. Gurdeep Raj, S. (2001). *Advanced Physical Chemistry*. Chennai: Goel Publishing Co., 25<sup>th</sup> Edition.
3. Bajpai, D.N., (2012). *Advanced Physical Chemistry*. New Delhi: S.Chand & Company Ltd., 1<sup>st</sup> Edition.
4. Rohatgi, K.K. & Mukherjee. (2008). *Fundamentals of Photochemistry*. New Jersey: Wiley Eastern, 1<sup>st</sup> Edition.
5. Dash, U.N. (1996), *A Text Book of Biophysical Chemistry*. New Delhi: Macmillan India Ltd, 1<sup>st</sup> Edition.

6. Upadhyay, L.B. & Laidler, K.J. (1998). *Physical chemistry with Biological Applications*. New Delhi: S.Chand & Company Ltd., 1<sup>st</sup> Edition.

### REFERENCES BOOKS

- Laidler, K.J. (2012). *Chemical Kinetics*. London: Harper International Edn., 3<sup>rd</sup> Edition.
- McQuarrie, D.A. & Simon, J.D. (1998). *Physical Chemistry- A Molecular Approach*, New Delhi: Viva Books (P) Ltd., 1<sup>st</sup> Edition.
- Atkins, P.W.(2000). *Physical Chemistry*. London: ELPS and Oxford University Press, , 6<sup>th</sup> Edition.
- Gurtu & Gurtu, J.N. *Biophysical Chemistry*. Meerut: Pragati Prakashan Publishers, 2<sup>nd</sup> Edition.
- Upadhyay & Nath, *Biophysical chemistry*. New Delhi: S.Chand & Company Ltd., 2<sup>nd</sup> edition.
- Jain, J.L.(1996). *Fundamentals of Biochemistry*. Delhi: Himalaya Publishing House, 3<sup>rd</sup> Edition.
- Satyanarayana, U. (1999). *Biochemistry*. Calcutta: Books and Allied (P) Ltd., 1<sup>st</sup> Edition.

Course Code 20PCHC42	PO1		PO2	PO3		PO4	PO5	PO6	PO7	PO8
	PSO 1.a	PSO 1.b	PSO 2	PSO 3.a	PSO 3.b	PSO 4	PSO 5	PSO 6	PSO 7	PSO 8
CO1	H	M	M	H	H	H	M	M	M	L
CO2	H	M	M	H	H	H	M	M	M	L
CO3	H	M	M	H	H	H	M	M	M	H
CO4	H	M	M	H	H	H	M	M	M	H
CO5	H	M	M	H	H	H	M	M	M	H

Dr. J. Kavitha  
Head of the Department

Dr.J.Kavitha  
Dr.A.Anitha  
Course Designers



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**VIRUDHUNAGAR - 626 001**

**M.Sc. CHEMISTRY**  
**(2022-2023 onwards)**

Semester IV	<b>CHEMICAL KINETICS AND CATALYSIS, PHOTO, BIOPHYSICAL AND SUPRAMOLECULAR CHEMISTRY</b>	Hours/Week: 6	
Core Course 11		Credits: 5	
Course Code 20PCHC42N		Internal 40	External 60

**COURSE OUTCOMES**

On completion of the course, the students will be able to

- CO1: extend the fundamental concepts and theories of reaction rate in kinetics, surface, photo, biophysical and supramolecular chemistry. [K2]
- CO2: make use of the principle and applications of kinetics and catalysis, Biophysical, photo, surface and Supramolecular chemistry. [K3]
- CO3: develop advanced knowledge of catalysis, kinetics of complex reactions, Bioenergetics, Photo, biophysical and supramolecular Chemistry. [K3]
- CO4: analyze the concepts of the fast reactions, biomolecular techniques, self assembly in supramolecular chemistry, surface, biophysical and photo chemistry. [K4]
- CO5: evaluate about complex reactions, catalysis, photo chemistry, biomolecular study and molecular recognition. [K5]

**UNIT I**

**Chemical Kinetics**

Theories of reaction rates: Collision theory of bimolecular reaction, Activated Complex theory of bimolecular reaction-Eyring equation. Theory of unimolecular gaseous reactions-Lindemann, Hinshelwood, RRK, RRKM and Slater treatment.

Kinetics of reaction in solution - influence of solvent, ionic strength, and pressure on rate of the reactions in solution - Significance of volume and entropy of activation - Primary and secondary salt effect.

Kinetics of complex reactions – reversible reactions, consecutive reactions – Parallel reactions and Chain reactions - photochemical  $H_2 - Cl_2$  reaction.

Rice Herzfeld mechanism of dissociation of organic molecules viz. dissociation of ethane, decomposition of acetaldehyde –study of  $H_2 - O_2$  explosive reactions - Study of fast reactions: Relaxation methods-temperature and pressure jump methods - Stopped flow technique, flash photolysis and Crossed molecular beam method. (18 Hours)

## **UNIT II Surface Chemistry and Catalysis**

Adsorption-Physical and chemical adsorption – adsorption isotherms – Langmuir, Freundlich and B.E.T-Temkin adsorption isotherms – measurement of surface area from BET - Adsorption on liquid surface-surface tension-Gibbs's adsorption isotherm. Mechanism of surface reactions, unimolecular and bimolecular surface reactions, Langmuir – Hinshelwood mechanism for gases only.

Catalysis- acid – base catalysis - Bronsted catalysis law –heterogeneous catalysis- Enzyme catalysis – effect of substrate concentration- Michaelis – Menton equation-effect of pH and temperature on enzyme catalysis. (18 Hours)

## **UNIT III**

### **Photo Chemistry**

Photophysical processes in electronically excited molecule: Types of photophysical pathways- Radiationless transition-internal conversion and intersystem crossing-Fluorescence emission-Triplet state and Phosphorescence emission-Photophysical kinetics of unimolecular process-delayed fluorescence- effect of temperature on emission process.

Photophysical kinetics of bimolecular processes: Bimolecular collision and mechanism of fluorescence quenching-Kinetics of collisional quenching-Stern-Volmer equation – excimer and exciplexes formation. Photosynthesis - solar energy conversion and storage-Lasers in photochemical kinetics. (18 Hours)

## **UNIT IV**

### **Biophysical Chemistry**

Standard free energy change in biochemical reaction-conversion of ADP to ATP- Biological redox reactions-redox potential, redox reactions and free energy. Hydrophobic interaction and membrane- Hydrogen bond-Biological significance of pKa and pH.Active transport: Thermodynamic treatment of membrane transport, ion-driven and ATP driven active transport, Ion channel opening.

Technique for bio-molecular study: Principle and factors affecting electro-phoretic mobility – Types of electrophoresis - zone electrophoresis–Paper electrophoresis, cellulose acetate

electrophoresis, Gel electrophoresis and Capillary Electrophoresis, - Application of electrophoresis. (18 Hours)

#### UNITV

##### **Molecular recognition and Supramolecular Chemistry**

Introduction: Guest-Host interaction, Classification of receptors-cation, anion and neutral receptors, chelate effect and macrocyclic effect - Molecular Recognition:Cation recognition-Crown ethers and Cryptands as receptors – Anion receptors – porphyrins. Calixarene and Cyclodextrin as receptors.

Molecular self Assembly: Based on hydrogen bond, one-pot reaction. Synthesis of Catenanes and Rotaxanes. Formation of novel self-assemblies to be utilized for diversified applications including drug delivery, self-sortng materials, smart self-healing materials and bio-sensors in industry. Applications of supramolecules as electrochemical sensor, optical sensor and molecular switches and wires. (18 Hours)

#### **TEXT BOOKS**

1. Puri, B.R. Sharma, L.R. &Pathania, M.S. (2003). *Principles of Physical Chemistry*. Jalandhar, Delhi: (Millennium Edn.) Vishal Publishing Co.,1<sup>st</sup> Edition.
2. Gurdeep Raj, S.(2001). *Advanced Physical Chemistry*. Chennai: Goel Publishing Co., 25<sup>th</sup> Edition.
3. Bajpai, D.N.,(2012). *Advanced Physical Chemistry*. New Delhi: S.Chand& Company Ltd.,1<sup>st</sup> Edition.
4. Rohatgi, K.K.& Mukherjee. (2008). *Fundamentals of Photochemistry*. New Jersey: Wiley Eastern, 1<sup>st</sup> Edition.
5. Dash, U.N.(1996), *A Text Book of Biophysical Chemistry*.New Delhi: Macmillan India Ltd, 1<sup>st</sup> Edition.
6. Kalsi, P.S., (2017), *Biophysical Chemistry*, New Delhi, New Age International(P) Limited Publisher, 1<sup>st</sup> edition.
7. Asim K Das, Mahua Das,(2017) *An Introduction to Supramolecular Chemistry*, , West Bengal, CBS Publishers and Distributers (P) Limited, 1 st edition.

#### **REFERENCES BOOKS**

1. Laidler, K.J. (2012). *Chemical Kinetics*. London: Harper International Edn., 3<sup>rd</sup> Edition.
2. McQuarrie, D.A. & Simon, J.D. (1998). *Physical Chemistry- A Molecular Approach*, New Delhi: Viva Books (P) Ltd., 1<sup>st</sup> Edition.

3. Atkins, P.W.(2000). *Physical Chemistry*. London: ELPS and Oxford University Press, ,  
6<sup>th</sup> Edition.
4. Upadhyay &Nath, *Biophysical chemistry*. New Delhi: S.Chand& Company Ltd., 2<sup>nd</sup>  
edition.

Course Code 20PCHC42N	PO1		PO2	PO3		PO4	PO5	PO6	PO7	PO8
	PSO 1.a	PSO 1.b	PSO 2	PSO 3.a	PSO 3.b	PSO 4	PSO 5	PSO 6	PSO 7	PSO 8
CO 1	H	M	M	H	H	H	M	M	M	L
CO 2	H	M	M	H	H	H	M	M	M	L
CO 3	H	M	M	H	H	H	M	M	M	H
CO 4	H	M	M	H	H	H	M	M	M	H
CO 5	H	M	M	H	H	H	M	M	M	H

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Dr.N.Ramiladevi  
Course Designers



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**M.Sc. CHEMISTRY**

**(For those who join in the Academic Year 2020-2021)**

Semester IV	<b>NANO AND GREEN CHEMISTRY</b>	Hours/Week: 6	
Core Course 12		Credits: 5	
Course Code <b>20PCHC43</b>		Internal 40	External 60

**COURSE OUTCOMES**

On completion of the course, students will be able to

CO1: understand the basic concepts in nanochemistry and green chemistry. [K2]

CO2: apply various methods for synthesis of nano particles ,characterization nanomaterials, study of applications of nano particles,synthesis using green techniques. [K3]

CO3: apply the techniques of nano chemistry in nanoparticles synthesis, characterization, applications and green chemistry in designing the environmentally benign synthesis. [K3]

CO4: examine the different methods for synthesis of nanomaterials,Instrumentation of SEM, TEM, STM, properties of nano particles and their applications and design the synthesis of compounds by adopting principles of green chemistry. [K4]

CO5: predict the methods of synthesis of nano particles, size of nano particles,properties and applications of nanoparticles and evaluate the advantages of green synthesis. [K5]

**UNIT I Nanochemistry - an Overview:**

- a) Introduction and classification
- b) Synthesis of Nanomaterials:
  - i) Physical Approach – Arc-discharge method, Laser ablation, High-energy ball milling, Chemical vapour deposition, Aero-sol synthesis
  - ii) Chemical Approach – Sol-gel synthesis, microwave method, sonochemical process, Co-precipitation, Reverse micelles / micro emulsion method. (18 Hours)

**UNIT II Instrumentation and Characterization of Nanomaterials:**

- a) Structural characterization – Atomic structure, Crystallography, particle size determination using XRD techniques
- b) Spectroscopic techniques – UV and Raman spectroscopy
- c) Principles of electron microscopy – SEM, TEM, STM (18 Hours)

**UNIT III Properties and Applications of Nanomaterials:**

- a) Properties - mechanical - optical – electrical - magnetic
- b) Applications of nanomaterials
  - i) in energy sector – high energy density batteries
  - ii) in next generation computer technology: phosphors for high-definition TV, low-cost flat-panel displays
  - iii) for water purification and in food
  - iv) for environment – Elimination of pollutants
  - v) in Biomedical - Application of Nano-Electromechanical devices to Drug Delivery, and Nano Biosensors:
    - a) Types and Applications of Biosensors
    - b) Biosensor developments
    - c) Nanobiosensors in modern medicine (18 Hours)

**UNIT IV Introduction to Green Chemistry:**

- a. Definition - Twelve principles of green chemistry. Designing a Green synthesis – choice of starting materials, choice of reagents, choice of catalysts, choice of solvents.
- b. Green Solvents – Supercritical CO<sub>2</sub>, Ionic liquids, Water.
- c. Green Catalysts – Acid catalysts, Oxidation catalysts, Basic catalysts, Polymer supported catalysts
- d. Phase-Transfer Catalysis in Green Synthesis – Introduction, Applications of PTC in Organic Synthesis. (18 Hours)

**UNIT V Synthesis involving basic principles of Green Chemistry:**

- a. Synthesis of Adipic acid, Catechol, BHT, Methyl methacrylate, Citral, Ibuprofen, Paracetamol, Furfural, Acetaldehyde, Urethane.
- b. Microwave Induced Green synthesis – Microwave Assisted Reactions in Water & Microwave Solvent Free Reactions.
- c. Ultrasound assisted green synthesis – Introduction, Esterification, Saponification, Hydrolysis, Oxidation, Reduction, Addition reactions, Substitution Reactions, Alkylations, coupling reactions. (18 Hours)

**TEXT BOOKS**

1. Pradeep, T. (2017). *Nano: The Essentials- Understanding Nanoscience and Nanotechnology*. New York: McGraw Hill Education (India) Private Limited., 1<sup>st</sup> Edition.
2. Charles Poole, P. Jr. Frank, J. (2017). *Introduction to Nanotechnology*. Nodia: Owens Wiley India Pvt. Ltd., 1<sup>st</sup> Edition.
3. Ahluwalia, V.K. (2013). *A Textbook of Green Chemistry*. New Delhi: Narosa Publishing House Pvt. Ltd., 1<sup>st</sup> Edition.
4. Ahluwalia, V.K. (2016). *Green Chemistry (Environmentally Benign Reactions)*. New Delhi: Ane Books Pvt. Ltd., 2<sup>nd</sup> Edition.
5. Kumar, V. (2010). *An Introduction to Green Chemistry*. Jalandhar: Vishal Publishing Co., 1<sup>st</sup> Edition.

**REFERENCE BOOKS**

1. Shah, M.A. & Tokeer Ahmed. (2013). *Principles of Nanoscience and Nanotechnology*. Delhi: Narosa Publishing House Pvt. Ltd., 1<sup>st</sup> Edition.
2. Subbiahbalaji. (2010). *Nanobiotechnology*. Chennai: MJP Publishers, 1<sup>st</sup> Edition.

3. Sanghi, R & Srivastava, M.M. (2003). *Green Chemistry (Environmental Friendly Alternatives)*. New Delhi: Narosa Publishing House, 1<sup>st</sup> Edition.
4. Desai, K.R. (2005). *Green Chemistry (Microwave Synthesis)*. Mumbai: Himalaya Publishing House, 1<sup>st</sup> Edition.

Course Code 20PCHC43	PO1		PO2	PO3		PO4	PO5	PO6	PO7	PO8
	PSO 1.a	PSO 1.b	PSO 2	PSO 3.a	PSO 3.b	PSO 4	PSO 5	PSO 6	PSO 7	PSO 8
CO1	H	H	M	H	H	M	H	M	M	H
CO2	H	H	M	H	H	M	H	M	M	H
CO3	H	H	M	H	H	M	H	M	M	H
CO4	H	H	M	H	H	M	H	M	M	H
CO5	H	H	M	H	H	M	H	M	M	H

Dr.J.Kavitha  
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**M.Sc. CHEMISTRY**

**(2022-2023 onwards)**

Semester IV	<b>NANO AND GREEN CHEMISTRY</b>	Hours/Week: 6	
Core Course -12		Credits: 5	
Course Code 20PCHC43N		Internal 40	External 60

### COURSE OUTCOMES

On completion of the course, students will be able to

- CO1: understand the basic concepts in nanochemistry and green chemistry. [K2]
- CO2: apply various methods for synthesis of nano particles ,characterization nanomaterials, study of applications of nano particles,synthesis using green techniques.[K3]
- CO3: apply the techniques of nano chemistry in nanoparticles synthesis, characterization, applications and green chemistry in designing the environmentally benign synthesis. [K3]
- CO4: examine the different methods for synthesis of nanomaterials, Instrumentation of SEM, TEM, STM, properties of nano particles and their applications and design the synthesis of compounds by adopting principles of green chemistry [K4]
- CO5: predict the methods of synthesis of nano particles, size of nano particles,properties and applications of nanoparticles and evaluate the advantages of green synthesis.[K5]

### UNIT I Nanochemistry - an Overview:

- a) Introduction : Nanomaterials and types-0D,1D,2D, nanowire, nanotubes.
- b) Synthesis of Nanomaterials: Top-down and Bottom –Up Approach
  - i) Physical Approach – Arc-discharge method, Laser ablation, High-energy ball milling, Chemical vapour deposition, Aero-sol synthesis

- ii) Chemical Approach – Sol-gel synthesis, microwave method, sonochemical process, Co-precipitation, Reverse micelles / micro emulsion method. (18 Hours)

**UNIT II Characterization and properties of Nanomaterials:**

- a) Structural characterization – Atomic structure, Crystallography, particle size determination using XRD techniques.
- b) Particle size and charge determination of nanomaterials – zeta potential.
- c) Properties - mechanical - optical – electrical - magnetic (18hours)

**UNIT III Applications of Nanomaterials:**

Applications of nanomaterials

- i) in energy sector – high energy density batteries
- ii) in next generation computer technology: phosphors for high-definition TV, low-cost flat-panel displays
- iii) for water purification and in food
- iv) for environment – Elimination of pollutants
- v) Medicinal applications of nanomaterials. (18hours)

**UNIT IV Introduction to Green Chemistry:**

- e. Definition - Twelve principles of green chemistry. Designing a Green synthesis – choice of starting materials, choice of reagents, choice of catalysts, choice of solvents.
- f. Green Solvents – Supercritical CO<sub>2</sub>, Ionic liquids, Water.
- g. Green Catalysts – Acid catalysts, Oxidation catalysts, Basic catalysts, Polymer supported catalysts
- h. Phase-Transfer Catalysis in Green Synthesis – Introduction, Applications of PTC in Organic Synthesis. (18hours)

**UNIT V Synthesis involving basic principles of Green Chemistry:**

- d. Synthesis of Adipic acid, Catechol, BHT, Methyl methacrylate, Citral, Ibuprofen, Paracetamol, Furfural, Acetaldehyde, Urethane.
- e. Microwave Induced Green synthesis – Microwave Assisted Reactions in Water & Microwave Solvent Free Reactions.
- f. Ultrasound assisted green synthesis – Introduction, Esterification, Saponification, Hydrolysis, Oxidation, Reduction, Addition reactions, Substitution Reactions, Alkylations, coupling reactions. (18hours)

**TEXT BOOKS**

1. Pradeep,T, (2017).*Nano: The Essentials- Understanding Nanoscience and Nanotechnology*. New York: McGraw Hill Education (India) Private Limited., 1<sup>st</sup> Edition.
2. Charles Poole, P. Jr. Frank ,J.(2017). *Introduction to Nanotechnology*.Nodia: Owens Wiley India Pvt. Ltd., 1<sup>st</sup> Edition.
3. Ahluwalia, V.K. ( 2013). *A Textbook of Green Chemistry*. New Delhi:Narosa Publishing House Pvt. Ltd., 1<sup>st</sup> Edition.
4. Ahluwalia, V.K. ( 2016). *Green Chemistry (Environmentally Benign Reactions)*. New Delhi: Ane Books Pvt. Ltd., 2<sup>nd</sup> Edition.
5. Kumar,V. (2010). *An Introduction to Green Chemistry*. Jalandhar: Vishal Publishing Co., 1<sup>st</sup> Edition.

**REFERENCE BOOKS**

1. Shah ,M.A.& Tokeer Ahmed .(2013). *Principles of Nanoscience and Nanotechnology*. Delhi: Narosa Publishing House Pvt. Ltd., 1<sup>st</sup> Edition.
2. Subbiahbalaji. (2010). *Nanobiotechnology*. Chennai: MJP Publishers, 1<sup>st</sup> Edition.
3. Sanghi, R &Srivastava, M.M. (2003).*Green Chemistry (Environmental Friendly Alternatives)*. New Delhi:Narosa Publishing House, 1<sup>st</sup> Edition.
4. Desai, K.R. (2005). *Green Chemistry (Microwave Synthesis)*. Mumbai: Himalaya Publishing House, 1<sup>st</sup> Edition.

Course Code 20PCHC43N	PO1		PO2	PO3		PO4	PO5	PO6	PO7	PO8
	PSO 1.a	PSO 1.b	PSO 2	PSO 3.a	PSO 3.b	PSO 4	PSO 5	PSO 6	PSO 7	PSO 8
CO 1	H	H	M	H	H	M	H	M	M	H
CO 2	H	H	M	H	H	M	H	M	M	H
CO 3	H	H	M	H	H	M	H	M	M	H
CO 4	H	H	M	H	H	M	H	M	M	H
CO 5	H	H	M	H	H	M	H	M	M	H

Dr.J.Kavitha  
Head of the Department

Dr. C. Vidyarani  
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Course Designers



# V.V.VANNIAPERUMAL COLLEGE FOR WOMEN

(Belonging to Virudhunagar Hindu Nadars)

An Autonomous Institution Affiliated to Madurai Kamaraj University, Madurai

Re-accredited with 'A' Grade (3<sup>rd</sup> Cycle) by NAAC

VIRUDHUNAGAR - 626 001

M.Sc. CHEMISTRY

(For those who join in the Academic Year 2020-2021)

Semester IV	<b>Inorganic Quantitative Analysis and Complex Preparation</b>	Hours/Week: 6	
Core Practical 4		Credits: 4	
Course Code <b>20PCHC41P</b>		Internal 40	External 60

## COURSE OUTCOMES

On completion of the course, the students will be able to

- CO1: separate and estimate mixtures of metal ions by volumetric and gravimetric methods. [K3]
- CO2: prepare coordination complexes such as Trithioureacopper(II) sulphate, potassium trioxalato aluminate(III), Tetramminecopper(II) sulphate, Reineck's salt. [K3]
- CO3: prepare coordination complexes such as *trans*-Potassium dioxalatodiaquachromate(III), *cis*-Potassium dioxalatodiaquachromate(III), Sodium trioxalato ferrate(III), Hexathiourealead(II) nitrate. [K3]
- CO4: examine the strengths of inorganic metal ions such as nickel, barium and zinc by gravimetric methods and compare the calculated strengths with the standard solutions. [K4]
- CO5: examine the strengths of inorganic metal ions such as iron(III), copper, calcium by volumetric methods and compare the calculated strengths with the standard solutions. [K5]

**1. Quantitative Analysis:** Separation and estimation of mixtures by volumetric and gravimetric methods. Some recommended mixtures are

- Estimation of Copper(V) and Nickel(G)
- Estimation of Copper (V) and Calcium(G)
- Estimation of Fe(III)(V) and Nickel (G)

- d. Estimation of Copper (V) and Barium(G)
- e. Estimation of Copper (V) and Zinc(G)
- f. Estimation of Calcium (V) and Copper(G)

## 2. Preparation of the following Inorganic complexes.

- a. Preparation of Trithioureacopper(II) sulphate
- b. Preparation of Potassium trioxalato aluminate(III)
- c. Preparation of Tetramminecopper(II) sulphate
- d. Preparation of Reineck's salt
- e. Preparation of *trans*-Potassium dioxalatodiaquachromate(III)
- f. Preparation of *cis*-Potassium dioxalatodiaquachromate(III)
- g. Preparation of Sodium trioxalato ferrate(III)
- h. Preparation of Hexathiourealead(II) nitrate

Course Code 20PCHC41P	PO1		PO2	PO3		PO4	PO5	PO6	PO7	PO8
	PSO 1a	PSO 1b	PSO 2	PSO 3a	PSO 3b	PSO 4	PSO 5	PSO 6	PSO 7	PSO 8
CO1	H	H	M	H	M	M	M	H	H	M
CO2	H	H	M	H	M	M	M	H	H	M
CO3	H	H	M	H	M	M	M	H	H	M
CO4	H	H	M	H	M	M	M	H	H	M
CO5	H	H	M	H	M	M	M	H	H	M

Dr. J. Kavitha  
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**VIRUDHUNAGAR - 626 001**

**M.Sc. CHEMISTRY**

**(For those who join in the Academic Year 2020-2021)**

Semester IV	<b>PROJECT VIVA-VOCE</b>	Hours/Week: 6	
Core Project		Credits: 5	
Course Code <b>20PCHC41PR</b>		Internal 40	External 60

## COURSE OUTCOMES

On completion of the course, the students will be able to

CO1: develop research methodologies along with literature survey. [K3]

CO2: categorize the synthesized materials using various analytical techniques. [K4]

CO3: interpret the analytical data and able to correlate theoretical and experimental results. [K4]

CO4: communicate the laboratory scientific results both in oral, written and electronic format to both chemists and non-chemists. [K4]

CO5: evaluate new methodologies to develop novel materials through new synthetic routes. [K5]

1. Each learner can select her research project in any one of the areas of chemistry in consultation with her guide and the Head of the department.
2. The project can be either developing novel materials through new synthetic routes or review of literature paper.
3. Either individual project or team work (only two students in a team) shall be chosen.
4. The project report should be submitted to the Principal through the Head of the Department of chemistry one week prior to the commencement of the summative examinations. If a candidate fails to submit her project report on the date presented above, she may be permitted to submit the same four days prior to the date of *Viva-voce* examination with a fine as prescribed by the college.
5. Each learner shall submit 2 copies of her project report for valuation.
6. The project report shall contain at least 25 pages excluding bibliography and appendices.

7. The project report shall be valued for a total of 100 marks out of which the external examiner and guide share 60 and 40 marks respectively. The sum of marks awarded by both the examiners shall be considered to be the final mark. Further for a pass in this paper as a whole a learner should secure at least 60 marks in project report and viva-voce put together.
8. If the learner fails to get the minimum pass mark in the project report, she shall be permitted to resubmit her project report once again within a period of 3 months after the publication of the result.

Course Code 20PCHC4PR	PO1		PO2	PO3		PO4	PO5	PO6	PO7	PO8
	PSO 1.a	PSO 1.b	PSO 2	PSO 3.a	PSO 3.b	PSO 4	PSO 5	PSO 6	PSO 7	PSO 8
CO1	H	M	M	H	H	H	M	M	M	H
CO2	H	M	M	H	H	H	M	M	M	H
CO3	H	M	M	H	H	H	M	M	M	H
CO4	H	M	M	H	H	H	M	M	M	H
CO5	H	M	M	H	H	H	M	M	M	H

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**VIRUDHUNAGAR - 626 001**

### M.Sc. CHEMISTRY

(2022-2023 onwards)

Semester IV	<b>Project - Research Methodology &amp; Ethics</b>	Hours/Week: 6	
Core Project		Credits: 5	
Course Code <b>22PCHC41PR</b>		Internal 60	External 40

### COURSE OUTCOMES

On completion of the course, the students will be able to

CO1: understand the fundamentals of research methodologies and develop ability to choose methods appropriate to research aims and objectives [K3]

CO2: select and define appropriate research problem [K4]

CO3: analyze various methods for collecting primary and secondary data along with literature Survey. [K4]

CO4: analyze research ethical issues related to Research and Publication. [K4]

CO5: evaluate new methodologies to develop novel materials through new synthetic routes. [K5]

#### Unit-I: Art of Research planning

Objectives of research – Understanding research and its goals. Critical thinking. Research topic selection and justification. Techniques involved in designing a questionnaire – Methods of scientific enquiry – formulation of hypotheses and testing of the same – Development of a research proposal – Theoretical and Experimental Processes. (6 hours)

#### Unit-II: Literature survey, Research sources

Sources of information- Literature search: Computers in literature search using Internet websites, Online data bases – search tools. Literature review – Case studies, review articles and Meta analysis – record of research review. Ethical and Moral Issues in Research, Plagiarism, tools to avoid plagiarism – Thesis writing, and Research report writing and

preparation of dissertation. Role of the librarian: ACS-pubs, Royal Society, Springer link, science direct, Wiley – Interscience. Submission of research articles for Publication to Reputed journals- h-index, i-index, ISSN, ISBN –Science Citation Index - chemistry journal index . Intellectual Property Rights – Copy right laws – Patent rights. (6 hours)

#### Project General Rules:

1. Each learner can select her research project in any one of the areas of chemistry in consultation with her guide and the Head of the department.
2. Course comprises two units Research Methodology theory paper and Project Completion.
3. An Internal Assessment for a maximum of 20 marks will be carried out for the theory paper.
- 4 The project can be either developing novel materials through new synthetic routes or review of literature paper.
- 5 Either individual project or team work (only two students in a team) shall be chosen.
- 6 The project report should be submitted to the Principal through the Head of the Department of chemistry one week prior to the commencement of the summative examinations. If a candidate fails to submit her project report on the date presented above, she may be permitted to submit the same four days prior to the date of *Viva-voce* examination with a fine as prescribed by the college.
- 7 Each learner shall submit 2 copies of her project report for valuation.
- 8 The project report shall contain at least 25 pages excluding bibliography and appendices.
- 9 The project report shall be valued for a total of 100 marks out of which the external examiner and guide share 40 and 60 marks respectively. The sum of marks awarded by both the examiners shall be considered to be the final mark. Further for a pass in this paper as a whole a learner should secure at least 60 marks in project report and viva-voce put together.
- 10 If the learner fails to get the minimum pass mark in the project report, she shall be permitted to resubmit her project report once again within a period of 3 months after the publication of the result.

#### References

1. Ganesan R (2011), *Research Methodology for Engineers* , MJP Publishers, Chennai.
2. Walpole R.A., Myers R.H., Myers S.L. and Ye, King (2007): *Probability & Statistics for Engineers and Scientists*, Pearson Prentice Hall, Pearson Education, Inc..
3. Anderson B.H., Dursaton, and Poole M(1997).: *Thesis and assignment writing*, Wiley Eastern.

4. Bjorn Gustavii: *How to write and illustrate scientific papers?* Cambridge University Press.
5. Bordens K.S. and Abbott, B.b.( 2008) *Research Design and Methods*, Mc Graw Hill.
6. Graves N, Varma V(199) *Working for a doctorate* Toutledge 7.
7. Graziano, A., M., and Raulin, M.,L (2007)*Research Methods – A Process of Inquiry*, Sixth Edition, Pearson.
8. Leedy., P., D.( 2005),*Practical Research – Planning and Design*, Eighth Edition, Pearson.
9. Kothari C.K (2004), *Research Methodology- Methods and Techniques*, New Age International, New Delhi.

Course Code 22PCHC41PR	PO1		PO2	PO3		PO4	PO5	PO6	PO7	PO8
	PSO 1.a	PSO 1.b	PSO 2	PSO 3.a	PSO 3.b	PSO 4	PSO 5	PSO 6	PSO 7	PSO 8
CO 1	H	M	M	H	H	H	M	M	M	H
CO 2	H	M	M	H	H	H	M	M	M	H
CO 3	H	M	M	H	H	H	M	M	M	H
CO 4	H	M	M	H	H	H	M	M	M	H
CO 5	H	M	M	H	H	H	M	M	M	H

Evaluation Pattern (100 marks)					
Internal Assessment (60marks)				External Assessment (40 marks)	
One Periodic Test (20)	Project Report (20)	Pre-Submission Presentation (10)	One Open online Course related to the Project (10)	Project Presentation (30)	Viva Voce (10)

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