

SRI KALISWARI COLLEGE (AUTONOMOUS), SIVAKASI
(AFFILIATED TO MADURAI KAMARAJ UNIVERSITY, MADURAI)
RE-ACCREDITED WITH 'A' GRADE (THIRD CYCLE) BY NAAC WITH CGPA 3.11)



Programme Scheme, Scheme of Examination and Syllabi
(From 2021-2022 Batch onwards)

Department of Chemistry

PG Programme

Approved in the Academic Council – XIII held on 11/08/2021

Curriculum Design and Development Cell
Annexure L

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HOD

**Dean of
Pure Science**

**Dean of
Academic Affairs**

Principal

SRI KALISWARI COLLEGE (AUTONOMOUS), SIVAKASI
DEPARTMENT OF CHEMISTRY
MEMBERS OF BOARD OF STUDIES

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2.	University Nominee	Dr.R.Mayil Murugan, Assistant Professor, Department of Physical Chemistry, Madurai Kamaraj University, Madurai – 625021 Phone : 9943041049 Mail id: ramamayil@gmail.com
3.	Academic Expert 1.	Dr.T.Esakki Durai, Principal Incharge & Associate Professor, Department of Chemistry, Devanga Arts College (Autonomous), Aruppukottai. Phone: 9442056667. Mail id: dacted@gmail.com
4.	Academic Expert 2.	Dr. S. Arunachalam, Associate Professor, Department of Chemistry, Kalasalingam Academy of Research and Education (Deemed to be University), Krishnankoil-626126, Phone: +91 9894575621 Mail id: drarunachalam.s@gmail.com
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8.	Mrs. M. Murugalakshmi	Assistant Professor of Chemistry
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11.	Mrs. R. Vijayalekshmi	Assistant Professor of Chemistry
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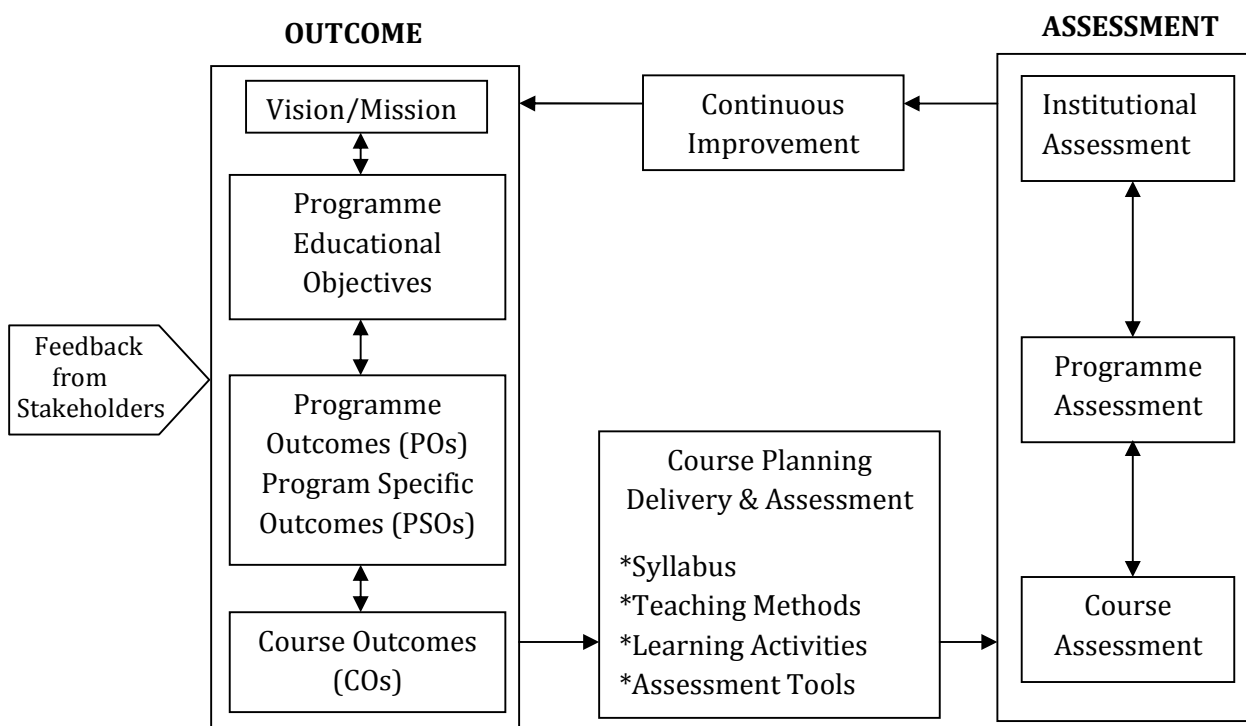
SRI KALISWARI COLLEGE (AUTONOMOUS), SIVAKASI
(Affiliated to Madurai Kamaraj University, Re-accredited with A Grade (CGPA 3.11) by NAAC)
DEPARTMENT OF CHEMISTRY
PG Programme – M. Sc Chemistry
GUIDELINES FOR OUTCOME-BASED EDUCATION WITH CHOICE BASED CREDIT SYSTEM
(From 2021-2022 Batch onwards)

INTRODUCTION

Sri Kaliswari College in its pursuit of imparting quality education has marked a remarkable growth in terms of academic excellence, infrastructure, student strength, ICT facilities, library and placement records since its establishment in 2000-2001. This institution constitutes an academic community that is committed to encourage the student community to experience and share knowledge, identify their potential, enhance the employability skills and enable them to pursue their goals. After the conferment of autonomous status in the year 2012, the college has so far gone for revision of the syllabi three times and is continually updating the syllabi to meet the needs and demands of the student community.

The institution in its success journey of imparting quality education has been Re-Accredited with A grade with (CGPA 3.11) in its third cycle of accreditation by NAAC. As an added feather to its cap, the institution has taken a giant leap to embrace the Outcome-Based Education system to enable the student community to develop their knowledge, skill and attitude simultaneously through a focused learning and help the graduates to compete with their global counterparts and prepare them for life.

I. OUTCOME-BASED EDUCATION (OBE) FRAMEWORK



II. VISION OF THE INSTITUTION

- To impart quality higher education to produce highly talented youth capable of developing the nation

III. MISSION OF THE INSTITUTION

- Ensuring quality in all aspects of the activities
- Developing the latent skills of the rural youth
- Providing value - based education to instill courage and confidence
- Nurturing the entrepreneurial skills of the rural youth
- Creating competency to meet global challenges
- Imbibing social awareness and social responsibilities

IV. VISION OF THE DEPARTMENT

- To produce quality chemistry professional with technical skill and applied knowledge to pursue higher education and research and to fulfill the jobs/employment opportunities in industries, scientific projects and allied sectors at regional and national levels.

V. MISSION OF THE DEPARTMENT

- To provide an academically sound environment that ensures understanding of key chemical concepts, principles and theories and cognitive development of students in a holistic manner.
- To provide knowledge and skills to the students thus enabling them to undertake further studies in chemistry related areas or multidisciplinary areas that can be helpful for self-employment/entrepreneurship.
- To mould a responsible citizen who is aware of most basic domain-independent knowledge, including critical thinking and communication.

VI. PROGRAMME EDUCATIONAL OBJECTIVES (PEOs)

The Graduates will

PEO1: achieve advance in-depth knowledge of chemistry and can pursue research programme in national and international level institution.

PEO2: able to identify, formulate, analyze synthesis and interpret various chemical compounds with modern instrumentation techniques to satisfy the needs of the society and the industries.

PEO3: equip with skills in research, critical thinking and analytical area.

PEO4: strengthen professional attitude with ethical values to enhance entrepreneurial skills.

PEO5: develop creativity, inventiveness, leadership and lifelong learning to become a successful professional.

VII. PROGRAMME OUTCOMES (POs)

P01: Disciplinary knowledge

Acquire comprehensive and scientific knowledge in the field of science.

P02: Critical thinking, Problem solving and Analytical reasoning

Engage in critical investigation through principle approaches or methods and draw realistic conclusions of problems by employing highly developed analytical and quantitative skills.

P03: Scientific reasoning and Research related skills

Ability to analyze, draw conclusions from qualitative/quantitative data and critically evaluate ideas and also acquire necessary research skills to carry out an experiment or investigation.

P04: Communication skills and Digital literacy

Communicate effectively on scientific achievements, basic concepts and recent developments with society at large and make use of appropriate software to prepare project report.

P05: Ethics, Values and Multicultural competence

Embrace ethical principles in all their activities, commit to professional and research ethics and practice tolerance and respect differences.

P06: Team Work, Leadership and Employability skills

Recognize the opportunities and contribute positively in collaborative scientific research and acquire the pre-requisite skills required for placements and higher education.

P07: Self-directed and Life-long learning

Recognize the need for engaging in independent and life-long learning in the emerging areas of the field of specialization.

VIII. PROGRAMME SPECIFIC OUTCOMES (PSOs) – M.Sc. CHEMISTRY

On successful completion of B.Sc. Chemistry, the students will

PSO1: acquire comprehensive knowledge and understanding of both theoretical and experimental/applied chemistry knowledge in various fields like Analytical chemistry, Physical Chemistry, Inorganic Chemistry, Organic Chemistry, Material chemistry, etc.

PSO2: develop skills to identify chemistry related problems, analysis and application of data using appropriate methodologies.

PSO3: design scientific experiments through statistical hypothesis testing, appropriate questions, planning and reporting experimental investigation.

PSO4: communicate effectively the concepts through technical writing as well as through oral presentation and acquire the ability to work in chemical simulation software and related computational work.

PSO5: embrace moral and research ethics, including fair benefit sharing, plagiarism, scientific misconduct and so on and develop the ability to spot data fabrication and fake news by applying rational skepticism and analytical reasoning.

PSO6: act as a team player by contributing in laboratory, field based situation and industry by acquiring technical, communicative, problem solving, intellectual and leadership skills.

PSO7: engage in independent and lifelong learning through use of advanced ICT techniques for personal academic growth as well as for increasing employability opportunity.

IX. PO-PSO Mapping Matrix – M.Sc. Chemistry

PO \ PSO	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7
P01	✓						
P02		✓					
P03			✓				
P04				✓			
P05					✓		
P06						✓	
P07							✓

X. PO-PEO Mapping Matrix – M.Sc. Chemistry

PO \ PEO	PEO1	PEO2	PEO3	PEO4	PEO5
P01	✓	✓	✓		
P02		✓	✓		✓
P03		✓	✓	✓	✓
P04		✓		✓	
P05			✓	✓	✓
P06			✓	✓	✓
P07		✓			✓

SRI KALISWARI COLLEGE (AUTONOMOUS), SIVAKASI
(Affiliated to Madurai Kamaraj University, Re-accredited with A Grade (CGPA 3.11) by NAAC)
DEPARTMENT OF CHEMISTRY
PG Programme - M.Sc. Chemistry

REGULATIONS

Duration of the Programme : Two years (equivalent to four semesters)

Eligibility

Candidate should have passed B. Sc. Chemistry or any other degree accepted by the Syndicate of the Madurai Kamaraj University, Madurai as its equivalent.

Medium of Instruction : English

Age Limit

Maximum age limit : No Age limit

Transitory Permission

Students joined from 2021 - 2023 may be permitted to write their examinations in this pattern up to April 2026.

SRI KALISWARI COLLEGE (AUTONOMOUS), SIVAKASI
DEPARTMENT OF CHEMISTRY
PG Programme – M.Sc. Chemistry
SCHEME OF EXAMINATION

For both UG and PG Programmes, the Internal and External marks are distributed as follows:

For all Theory Courses : Internal Marks: 40; External Marks: 60

For all Practical Courses and Project : Internal Marks: 50; External Marks: 50

Internal Mark Distribution for Theory Courses

Assessment Type	Marks	Scheme of Assessment
Internal Test	15 marks	Two Internal Tests and 1 Model Exam will be conducted and average of the best two will be considered
Written Assignment/ E-Assignment/ Case Studies/ Reviews/ Field Assignments/ Poster Presentations/ Portfolios	5 marks	Any one of the Assignments will be given
Quiz	5 marks	One Quiz Test will be conducted
Viva/ Oral Exam/ Group discussion/ Role Play	10 marks	Test will be conducted in any one of the Oral Mode
Seminar	5 marks	One Seminar for each course

Internal Mark Distribution for Practical Courses

Assessment Type	Marks	Scheme of Assessment
Lab work/Program Execution	40 marks	Two Internal Tests will be conducted and the average of the two will be considered
Observation/Record Notebook	5 marks	Assessment will be done during every practical class
Viva –Voce / Lab Quiz	5 marks	Two Lab Quiz Tests/viva-voce will be conducted and the average of the two will be considered

External Mark Distribution for Practical Courses

Assessment Type	Marks	Scheme of Assessment
Lab work/Program Execution	40 marks	End result of the Practical
Viva –Voce	10 marks	Oral Mode Test

SRI KALISWARI COLLEGE (AUTONOMOUS), SIVAKASI
DEPARTMENT OF CHEMISTRY
PG Programme – M.Sc. Chemistry
QUESTION PAPER PATTERN

Internal Test – 40 Marks - 1 hr 45 mins Duration

S.No	Type of Questions	Marks
1.	Objective type Questions Multiple Choice – 4 questions Answer in a Word/Sentence – 4 questions	04 04
2.	Short Answer –3 questions – either or type	3x4=12
3.	Long Answer–2 questions – either or type	2x10=20

Summative Examinations – 60 Marks -3 hrs Duration

S.No	Type of Questions	Marks
1.	Objective type Questions: Multiple Choice – 5 questions Answer in a Word/Sentence – 5 questions	05 05
2.	Short Answer 5 questions – either or type	5x4=20
3.	Long Answer 3 questions – either or type	3x10=30

SRI KALISWARI COLLEGE (AUTONOMOUS), SIVAKASI
DEPARTMENT OF CHEMISTRY
PG Programme - M.Sc. Chemistry

Attainment of Course outcomes

Attainment of Course outcomes is computed using Direct and Indirect assessment methods. Direct Method of Assessment is based on performance of the students in the Continuous Internal Assessment Tests, Summative Examinations and supporting activities such as Seminar, Assignment, Case study, Group Discussion, Quiz, etc., and Indirect Method of Assessment is based on periodical feedback from the students at the end of each course.

Weightage of Direct and Indirect Assessment in computation of attainment of each course is 70% for Direct Assessment and 30% for Indirect Assessment.

Direct Assessment of Course outcome attainment

i) Rubrics:

Internal Assessment contributes 60% and Summative Examinations Assessment contributes 40% to the Direct Assessment of a course outcome for Theory Courses. For the Practical Courses, Internal Assessment contributes 70% and Summative Examinations Assessment contributes 30% to the Direct Assessment of a course outcome.

ii) Setting of Target:

50% of the maximum mark is set as target of Internal Assessment tools and the average mark of the class is set as target of Summative Examinations Assessment.

Formula for calculating percentage attainment of each course outcome

Based on the result of Summative Examinations and Internal Assessment tools, the number of students scoring more than the target is found out.

For each Internal Assessment Tools,

$$\text{Percentage attainment of each course outcome} = \frac{\text{No. of Students who scored more than the target in the concerned course outcome}}{\text{Total Number of Students}} \times 100$$

$$\begin{array}{lcl} \text{Percentage attainment of each} & & \text{Average of percentage attainment of} \\ \text{Course outcome for Internal} & = & \text{all Internal Assessment tools} \\ \text{Assessment tools} & & \end{array}$$

For Summative Examinations,

$$\text{Percentage attainment of each Course outcome} = \frac{\text{No. of Students who scored more than the target in the concerned co}}{\text{Total Number of Students}} \times 100$$

Formula for calculating Attainment Percentage of Course outcome of a course

$$\text{Percentage Attainment of Course outcome for Internal Assessment tools} = \text{Average of percentage attainment of all COs}$$

$$\text{Percentage Attainment of Course outcome for Summative Examinations} = \text{Average of percentage attainment of all COs}$$

Final Direct Assessment of Course outcome Attainment

For Theory Courses

$$\text{Percentage Attainment of Course outcome through Direct Assessment} = (0.6 \times \text{percentage attainment of CO for internal assessment tool}) + (0.4 \times \text{percentage attainment of CO for summative examinations})$$

For Practical Courses

$$\text{Percentage Attainment of Course outcome through Direct Assessment} = 0.7 \times \text{percentage attainment of CO for Internal Assessment tools} + 0.3 \times \text{percentage attainment of CO for Summative Examinations}$$

Indirect Assessment of CO Attainment

The course outcome feedback is conducted at the end of every semester by distributing structured feedback questionnaire to the students. The analysis of this feedback questionnaire is done on the following score. The feedback forms will be sorted with various scores and feedbacks with a score more than 5.5 are considered as satisfactory level for calculations for indirect attainment.

A : 10-8.5 B : 8.4-7.0 C : 6.9-5.5 D : 5.4-4.0 E : 3.9-0

$$\text{Percentage attainment for each CO} = \frac{\text{Satisfaction Number}}{\text{Response Received}} \times 100$$

Percentage Attainment of CO of a course = Average of percentage attainment of all Cos

Final Assessment of CO attainment

$$\text{Average course attainment} = 0.7 \times \text{Direct assessment of CO attainment} + 0.3 \times \text{Indirect assessment of CO attainment}$$

Expected Level of Attainment for each of the Course Outcomes

CO	Level of Attainment
Above 70%	Excellent
60 -70 %	Very good
50-60 %	Good
40 – 50 %	Satisfactory
Below 40%	Not Satisfactory

Assessment of PO attainment

At the end of the each programme, the Direct PO Assessment is done from the CO Attainment of all courses. The Direct PO Attainment for a particular course is determined from the attainment values obtained for each course outcome related to that PO and the CO-PO mapping values.

$$\text{Weighted contribution of the course in attainment of each PO} = \frac{\text{Weighted Percentage of contribution of the course in attainment of each PO}}{\text{average course attainment}} \times 100$$

Expected Level of Attainment for each of the Programme Outcomes

PO	Level of Attainment
Above 70%	Excellent
60 -70 %	Very good
50-60 %	Good
40 – 50 %	Satisfactory
Below 40%	Not Satisfactory

Attainment of Programme Educational Objectives (PEO)

PEOs are assessed after 3 to 4 years of graduation. Attainment is measured based on the Feedback from Stakeholders

1. Alumni
2. Parents
3. Employer

The analysis of this feedback questionnaire is done on the following score. The feedback forms will be sorted with various scores and feedbacks with a score more than 5.5 are considered as satisfactory level for calculations for Indirect Attainment.

A : 10-8.5 B : 8.4-7.0 C : 6.9-5.5 D : 5.4-4.0 E : 3.9-0

$$\text{Percentage attainment of PEOs} = \frac{\text{Satisfaction number}}{\text{Response Received}} \times 100$$

Expected Level of Attainment for each of the Programme Educational Objectives

PEO	Level of Attainment
Above 70%	Excellent
60 -70 %	Very good
50-60 %	Good
40 – 50 %	Satisfactory
Below 40%	Not Satisfactory

SRI KALISWARI COLLEGE (AUTONOMOUS), Sivakasi
DEPARTMENT OF CHEMISTRY
PG Programme - M.Sc. Chemistry
CURRICULUM STRUCTURE
OUTCOME-BASED EDUCATION WITH CHOICE BASED CREDIT SYSTEM
(From 2021-2022 Batch onwards)

Subject	Sem I	Sem II	Sem III	Sem IV	Credits
Core Courses	6 (5) 6 (5) 6P (5) 6P (4)	6 (5) 6 (5) 6P (5) 6P (4)	6 (5) 6 (5) 6P (5) 6P (4)	5 (5) 5 (5) 5 (4)	71
Elective Courses	6 (4)	-	6 (4)	--	8
Non -Major Elective Course	--	6 (4)	--	--	4
Self-paced Learning (Swayam Course)	--		(3)	--	3
Project	--	--	--	15 (4)	4
Total Hours /Credits (Per week)	30 (23)	30 (23)	30 (26)	30 (18)	90 120

SRI KALISWARI COLLEGE (AUTONOMOUS), Sivakasi
DEPARTMENT OF CHEMISTRY
PG Programme - M.Sc. Chemistry
CURRICULUM PATTERN
OUTCOME-BASED EDUCATION WITH CHOICE BASED CREDIT SYSTEM
(From 2021-2022 Batch onwards)
PROGRAMME CODE – PCH

Semester	Course Code	Course Name	Hours	Credits
I	21PCHC11	Core Course - I: Reaction Mechanism and Stereochemistry	6	5
	21PCHC12	Core Course - II: Structure and Bonding	6	5
	21PCHC13	Core Course - III: Electrochemistry, Thermodynamics and Surface chemistry	6	5
	21PCHC1P	Core Course - IV: Practical: Organic Quantitative and Qualitative Analysis	6	4
	21PCH011 21PCH012 21PCH013	Elective Course - I: 1. Green Chemistry 2. Material Chemistry 3. Medicinal and Pharmaceutical Chemistry	6	4
	Total		30	23
II	21PCHC21	Core Course - V: Rearrangement, Name Reactions, Oxidation and Reduction	6	5
	21PCHC22	Core Course -VI: Coordination, Bioinorganic and Inorganic Photochemistry	6	5
	21PCHC23	Core Course - VII: Group Theory, Equilibria and Statistical Thermodynamics	6	5
	21PCHC2P	Core Course - VIII: Practical: Inorganic Quantitative and Qualitative Analysis	6	4
	21PCHN21	Non-Major Elective Course: Chemistry for Healthy Living	6	4
	Total		30	23
III	21PCHC31	Core Course - IX: Spectroscopy and Spectrometry	6	5
	21PCHC32	Core Course - X: Nuclear, Organometallics and Inorganic Spectroscopy	6	5
	21PCHC33	Core Course - XI: Spectroscopy and Photochemistry	6	5
	21PCHC3P	Core Course - XII: Practical: Physical Chemistry	6	4
	21PCH031	Elective Course- II: 1. Nuclear Reactions, Radiation Chemistry, Photoelectron Spectroscopy and Organometallics in	6	4

	21PCH032	Industry		
	21PCH033	2. Advanced Analytical Chemistry		
		3. Drug Design and Discovery		
	21PCHM31	Self-paced Learning (Swayam Course)		
		1. Advanced Transition Metal Organometallic Chemistry		3
	21PCHM32	2. Chemistry of Main Group Elements		
Total			30	26
IV	21PCHC41	Core Course - XIII: Photochemistry, Pericyclic Reactions, Heterocycles and Natural Products	5	5
	21PCHC42	Core Course - XIV: Quantum and Chemical Kinetics	5	5
	21PCHC43	Core Course - XV: Research Methodology	5	4
	21PCHJ41	Core Course - XVI: Project	15	4
Total			30	18

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DEPARTMENT OF CHEMISTRY
UG Programme - M.Sc. Chemistry
OUTCOME-BASED EDUCATION WITH CHOICE BASED CREDIT SYSTEM
 (From 2021-2022 Batch onwards)

PROGRAMME ARTICULATION MATRIX (PAM)

Semester	Course Code	Course Name	PO1	PO2	PO3	PO4	PO5	PO6	PO7
I	21PCHC11	Core Course - I: Reaction Mechanism and Stereochemistry	15	12	8	5	4	4	2
	21PCHC12	Core Course - II: Structure and Bonding	15	12	8	5	3	4	3
	21PCHC13	Core Course - III: Electrochemistry, Thermodynamics and Surface chemistry	15	12	8	5	4	4	3
	21PCHC1P	Core Course - IV: Practical: Organic Quantitative and Qualitative Analysis	15	12	8	5	4	4	2
	21PCHO11 21PCHO12 21PCHO13	Elective Course - I: 1. Green Chemistry 2. Material Chemistry 3. Medicinal and Pharmaceutical Chemistry	15	12	8	5	4	4	3
II	21PCHC21	Core Course - V: Rearrangement, Name Reactions, Oxidation and Reduction	15	13	7	5	4	4	2
	21PCHC22	Core Course - VI: Coordination, Bioinorganic and Inorganic Photochemistry	15	12	8	5	4	3	2
	21PCHC23	Core Course - VII: Group Theory, Equilibria and Statistical Thermodynamics	15	12	8	5	4	3	2
	21PCHC2P	Core Course - VIII: Practical: Inorganic	15	12	8	5	3	4	3

		Quantitative and Qualitative Analysis								
	21PCHN21	Non-Major Elective Course: Chemistry for Healthy Living	12	7	2	9	0	7	7	
III	21PCHC31	Core Course - IX: Spectroscopy and Spectrometry	15	12	8	5	4	4	3	
	21PCHC32	Core Course - X: Nuclear, Organometallics and Inorganic Spectroscopy	15	13	8	5	4	4	2	
	21PCHC33	Core Course - XI: Spectroscopy and Photochemistry	15	12	8	5	4	4	2	
	21PCHC3P	Core Course - XII: Practical: Physical Chemistry	15	13	8	5	4	4	3	
	21PCH031	Elective Course – II: 1. Nuclear Reactions, Radiation Chemistry, Photoelectron spectroscopy and Organometallics in Industry 2. Advanced Analytical Chemistry 3. Drug Design and Discovery	15	12	8	6	4	3	2	
	21PCH032									
	21PCH033									
	21PCHM31	Self-paced Learning (Swayam Course) 1. Advanced Transition Metal Organometallic Chemistry 2. Chemistry of Main Group Elements	15	12	8	7	3	2	5	
	21PCHM32									
IV	21PCHC41	Core Course - XIII: Photochemistry, Pericyclic Reactions, Heterocycles and Natural Products	15	13	10	5	4	3	4	
	21PCHC42	Core Course - XIV: Quantum and Chemical Kinetics	15	12	7	6	5	4	4	
	21PCHC43	Core Course - XV: Research Methodology	15	12	8	6	5	5	4	

	21PCHJ41	Core Course - XVI: Project	15	12	8	5	6	4	5
Total Weightage of all Courses Contributing to PO			297	239	154	109	77	78	63

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DEPARTMENT OF CHEMISTRY
UG Programme - M.Sc. Chemistry
OUTCOME-BASED EDUCATION WITH CHOICE BASED CREDIT SYSTEM
(From 2021-2022 Batch onwards)

PROGRAMME ARTICULATION MATRIX – WEIGHTED PERCENTAGE

Semester	Course Code	Course Name	P01	P02	P03	P04	P05	P06	P07
I	21PCHC11	Core Course - I: Reaction Mechanism and Stereochemistry	5.05	5.02	5.19	4.59	5.19	5.13	3.17
	21PCHC12	Core Course - II: Structure and Bonding	5.05	5.02	5.19	4.59	3.9	5.13	4.76
	21PCHC13	Core Course - III: Electrochemistry, Thermodynamics and Surface chemistry	5.05	5.02	5.19	4.59	5.19	5.13	4.76
	21PCHC1P	Core Course - IV: Practical: Organic Quantitative and Qualitative Analysis	5.05	5.02	5.19	4.59	5.19	5.13	3.17
	21PCHO11 21PCHO12 21PCHO13	Elective Course - I: 1. Green Chemistry 2. Material Chemistry 3. Medicinal and Pharmaceutical Chemistry	5.05	5.02	5.19	4.59	5.19	5.13	4.76
II	21PCHC21	Core Course - V: Rearrangement, Name Reactions, Oxidation and Reduction	5.05	5.44	4.55	4.59	5.19	5.13	3.17
	21PCHC22	Core Course -VI: Coordination, Bioinorganic and Inorganic Photochemistry	5.05	5.02	5.19	4.59	5.19	3.85	3.17
	21PCHC23	Core Course - VII: Group Theory, Equilibria and Statistical Thermodynamics	5.05	5.02	5.19	4.59	5.19	3.85	3.17

	21PCHC2P	Core Course - VIII: Practical: Inorganic Quantitative and Qualitative Analysis	5.05	5.02	5.19	4.59	3.9	5.13	4.76
	21PCHN21	Non-Major Elective Course: Chemistry for Healthy Living	4.04	2.93	1.3	8.26	0	8.97	11.11
III	21PCHC31	Core Course - IX: Spectroscopy and Spectrometry	5.05	5.02	5.19	4.59	5.19	5.13	4.76
	21PCHC32	Core Course - X: Nuclear, Organometallics and Inorganic Spectroscopy	5.05	5.44	5.19	4.59	5.19	5.13	3.17
	21PCHC33	Core Course - XI: Spectroscopy and Photochemistry	5.05	5.02	5.19	4.59	5.19	5.13	3.17
	21PCHC3P	Core Course - XII: Practical: Physical Chemistry	5.05	5.44	5.19	4.59	5.19	5.13	4.76
	21PCHO31	Elective Course- II: 1. Nuclear Reactions, Radiation Chemistry, Photoelectron spectroscopy and Organometallics in Industry 2. Advanced Analytical Chemistry 3. Drug Design and Discovery							
	21PCHO32		5.05	5.02	5.19	5.5	5.19	3.85	3.17
	21PCHO33								
	21PCHM31	Self-paced Learning (Swayam Course) 1. Advanced Transition Metal Organometallic Chemistry	5.05	5.02	5.19	6.42	3.9	2.56	7.94
	21PCHM32	2. Chemistry of Main Group Elements							
IV	21PCHC41	Core Course - XIII: Photochemistry, Pericyclic Reactions, Heterocycles and Natural Products	5.05	5.44	6.49	4.59	5.19	3.85	6.35
	21PCHC42	Core Course - XIV: Quantum and Chemical Kinetics	5.05	5.02	4.55	5.5	6.49	5.13	6.35

	21PCHC43	Core Course - XV: Research Methodology	5.05	5.02	5.19	5.5	6.49	6.41	6.35
	21PCHJ41	Core Course - XVI: Project	5.05	5.02	5.19	4.59	7.79	5.13	7.94
Total Weightage of all Courses Contributing to PO			100	100	100	100	100	100	100

SRI KALISWARI COLLEGE (AUTONOMOUS), SIVAKASI
DEPARTMENT OF CHEMISTRY
PG Programme – M.Sc. Chemistry
SEMESTER - I
CORE COURSE - I: REACTION MECHANISM AND STEREOCHEMISTRY
(21PCHC11)
(From 2021 – 2022 Batch onwards)

HOURS/WEEK: 6
CREDITS : 5
DURATION : 90 hrs

INT. MARKS : 40
EXT. MARKS : 60
MAX. MARKS : 100

Preamble

This course enables the students to acquire the knowledge in reaction mechanism, substitution reaction of aliphatic and aromatic compounds.

Course Outcomes (CO)

On successful completion of the course, the learners will be able to

- CO1[K2]:** explain reaction mechanism by kinetic and non-kinetic methods, substitution reactions using nucleophiles and electrophiles and stereochemistry
- CO2[K3]:** determine aromaticity and stereochemistry of organic molecules
- CO3[K4]:** compare the substituent effect through kinetic and non-kinetic methods, aromaticity and antiaromaticity and stereochemistry of mono and disubstituted cycloalkanes
- CO4[K5]:** deduce the mechanism of various types of nucleophilic substitution reaction and asymmetric synthesis
- CO5[K6]:** assimilate the knowledge of reaction intermediates and stereochemistry to propose a mechanism for the given reaction.

CO-PO Mapping table (Course Articulation Matrix)

PO CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1 [K2]	3	2	1	1	-	-	-
CO2 [K3]	3	2	1	1	1	1	-
CO3 [K4]	3	2	2	1	1	1	-
CO4 [K5]	3	3	2	1	1	1	1
CO5 [K6]	3	3	2	1	1	1	1
Weightage of the course	15	12	8	5	4	4	2
Weighted percentage of course contribution to POs	5.05	5.02	5.19	4.59	5.19	5.13	3.17

Based on the level of contribution ('3'-High, '2'-Medium, '1'-Low '-' No Correlation)

UNIT I - ALIPHATIC NUCLEOPHILIC SUBSTITUTION (18 hrs)

Mechanism of Nucleophilic Substitution Reactions: S_N^1 - S_N^2 - S_N^i
Mechanisms - Solvent and Leaving Group Effects - Neighbouring Group Participation (NGP) - Substitution at Carbonyl - Vinylic and Bridge head System - Substitution with Ambident Nucleophiles - "O" vs "C" Alkylation - Role of LDA, Crown Ethers and Phase Transfer Catalysts (PTC) in Nucleophilic Substitution Reactions - Generation of Enolates - Enolate Selectivity (Kinetic vs Thermodynamic) - Alkylation of Enolates - Stereochemistry of Enolate Alkylation - Mechanism of Ester Hydrolysis (only Bac^2 , Aac^2 And Aal^1) - Alkylation of Active Methylene Compounds - Asymmetric Alkylation (Evans, Enders and Meyers Procedures) - Preparation and Synthetic Utility of Enamines - Finkelstein Reaction - Wurtz Coupling.

UNIT II - AROMATIC ELECTROPHILIC AND NUCLEOPHILIC SUBSTITUTION REACTIONS (18 hrs)

Aromaticity: Aromaticity - Huckel's Rule - Antiaromaticity - Homoaromaticity - Alternant and Non-Alternant Hydrocarbons - Benzenoid and Non-Benzenoid Systems. **Aromatic Electrophilic Substitution:** Nitration - Sulfonation - Friedel - Crafts Alkylation and Acylation - Synthesis of Di- and Tri-Substituted Benzenes from Benzene or Mono-Substituted Benzenes - Haworth Reaction (For Naphthalene) - Scholl Reaction - Vilsmeier-Haack Formylation - Gattermann Reaction - Reimer - Tiemann - Bischler - Napieralski Reactions. **Aromatic Nucleophilic Substitution:** Meisenheimer Complex Mechanism - Benzyne Mechanism. Reactions of Aryldiazonium Salts: Zeigler Alkylation - Vicarious Nucleophilic Substitution (VNS) - Chichibabin - Schiemann Reactions.

UNIT III - STEREOCHEMISTRY (18 hrs)

Chirality: Symmetry Elements - Asymmetric and Dissymmetric Chiral Molecules - Calculation of Number of Optical Isomers. Compounds Containing Two Asymmetric Centers - Erythro and Threo Isomers. Conversion of Fischer Projection into Perspective Forms. Erythro and Threo - Inter Conversion of Fischer to Sawhorse and Newman Projections. Interpretation of Homotopic, Enantiotopic and Diastereotopic Atoms and Faces. Pro - Chiral Carbon. Concept of *Re*- and *Si*- Faces - R & S Nomenclature of Simple Compounds - Allenes - Spiranes and Biphenyls. Asymmetric Synthesis - Cram's Rule and Felkin - Anh Model. Conformational Analysis of Mono and Di-Substituted Cyclopropane - Cyclobutane - Cyclopentane - Cyclohexane - Decalin. Description of Various Types of Optically Active Compounds including Allenes - Cumulenes - Spiranes - Biphenyls - *Trans* - Cyclooctene.

UNIT IV - REACTION MECHANISM (18 hrs)

Kinetic and Non-Kinetic Methods: Inductive effect, electromeric effect Isolation and Trapping of Intermediates - Isotopic Labeling Studies - Primary

Kinetic Isotopic Effect –Generation of Kinetic and Thermodynamic Enolates. Hammett Equation – Taft Equation – Significance of Reaction with Substituent Constants - Applications –Ambident Nucleophiles – CN^- – NO_2^- – Phenoxide ion – Ambident Dianions.

UNIT V - REACTIVE INTERMEDIATES

(18 hrs)

Organic Reactive Intermediates: Generation, Stability and Reactivity of Carbocations – Friedel – Craft Reaction – Baeyer – Villiger Oxidation – Carbanions – Benzilic Acid Rearrangement – Perkin Reaction. Free Radicals – Sandmeyer Reaction – Wurtz-Fittig Reaction. Carbenes – Reimer-Tiemann Reaction – Carbenoids – Simmons – Smith Reaction. Nitrenes – Enamines – Selective Alkylation and Arylation of Ketones and Aldehydes – Phosphorous Ylides – Wittig Reaction

TEXTBOOKS

1. Finar. I. L. *Organic chemistry Vol II*. Pearson Education, 2001.
2. Jerry March. *Advanced Organic Chemistry*. John Wiley & Sons, 5th Ed., 2001.
3. Carey F. and Sundberg R. J. *Advanced Organic Chemistry-Part A and B*. Springer Science, 5th Ed., 2007.
4. Eliel E. L. and Wilen S.H. *Stereochemistry of Organic Compounds*. Wiley India, 2010.

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Books

1. Smith M. B. and Jerry March. *Advanced Organic Chemistry*. John Wiley & Sons, 5th Ed., 2001.
2. Clayden J., Greeves N. and Warren. S. *Organic Chemistry*. Oxford University Press, 2nd Ed., 2012.
3. Norman R. O. C. and Coxon. J. M. *Principles of Organic Synthesis*. Chapman & Hall, 3rd Ed., 1993.

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1. <https://nptel.ac.in/courses/104/101/104101115/>
2. <https://www.classcentral.com/course/swayam-stereochemistry-14305>
3. <https://nptel.ac.in/content/storage2/courses/104103022/download/module6.pdf>

SRI KALISWARI COLLEGE (AUTONOMOUS), SIVAKASI
DEPARTMENT OF CHEMISTRY
PG Programme – M.Sc. Chemistry
SEMESTER - I
CORE COURSE - II: STRUCTURE AND BONDING (21PCHC12)
(From 2021 – 2022 Batch onwards)

HOURS/WEEK: 6
CREDITS : 5
DURATION : 90 hrs

INT. MARKS : 40
EXT. MARKS : 60
MAX. MARKS : 100

Preamble

This course provides in-depth knowledge on chemical bonding and its application in various compounds, solid states, inorganic polymers, chain, cages and cluster compounds.

Course Outcomes (CO)

On successful completion of the course, the learners will be able to

- CO1[K1]:** describe the various concepts of bonding in covalent, ionic, inorganic polymers, chain, cages and cluster compounds
- CO2[K2]:** interpret weak chemical forces and packing in solid state
- CO3[K3]:** employ the concepts of hybridization, VB, VSEPR and MO theory to determine the shapes of various molecules in covalent, inorganic polymers, chain, cages and cluster compounds
- CO4[K4]:** discriminate the structure and defects of crystals
- CO5[K5]:** justify the structure and bonding of boranes, carboranes, metallocarboranes and metal clusters using Wade's Rule, Styx Number, isolobality and capping rule.

CO-PO Mapping table (Course Articulation Matrix)

CO \ PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1 [K1]	3	2	1	1	1	-	-
CO2 [K2]	3	2	1	1	1	1	1
CO3 [K3]	3	2	2	1	-	1	-
CO4 [K4]	3	3	2	1	-	1	1
CO5 [K5]	3	3	2	1	1	1	1
Weightage of the course	15	12	8	5	3	4	3
Weighted percentage of Course contribution to POs	5.05	5.02	5.19	4.59	3.9	5.13	4.76

Based on the level of contribution ('3'-High, '2'-Medium, '1'-Low '-' No Correlation)

UNIT I – CHEMICAL BONDING - I

(18 hrs)

V.B. Approach to Covalent Bonding: Heitler – London, Pauling – Slater Refinements – limitation – Concept of Hybridization – VSEPR Theory – limitation – Shapes of Molecules – Bent Rules – Electronegativity and Partial Ionic Character – **Molecular Orbital Approach to Covalent Bonding and its limitation:** Symmetry and Overlap of Atomic Orbitals – Symmetry of Molecular Orbitals – Sigma – Pi and Delta – Bondings – LCAO and MO Diagrams of Heteronuclear Diatomic (CO, NO, HF, HCl) molecules – Triatomic Molecules (H₂O, BeH₂, CO₂) – Polyatomic Molecules (NH₃) – Bond Length – Bond Order – Bond Energy – Walsh Diagram for H₂O and BeH₂ Bonds – Concept of Multicenter Bonding – Partial Ionic Character of Covalent Bonds.

UNIT II – CHEMICAL BONDING - II

(18 hrs)

Pseudo Halogen – Structure and Bonding in ClF₃, BrF₃, BrF₅, IF₅, IF₇. Oxides and Oxyacids of Halogens. Bonding in Noble Gas Compounds – XeCl₂, XeF₄, XeOF₄, XeF₆ - Ionic Bond – Lattice Energy – Born – Haber Cycle – Born-Landé Equations (Determination of Lattice Energy For NaCl) – Kapustinski Equation – Fajan's Rule – Effects of Polarization. Weak Chemical Forces – Ion-Dipole Forces – Dipole-Dipole Interaction – Induced Dipole Interaction – Instantaneous Dipole - Hydrogen Bonding.

UNIT III – SOLID STATE CHEMISTRY

(18 hrs)

Packing of Atoms and Ions : Close Packing of Atoms and Ions – FCC – HCP – BCC Types of Packing – Tetrahedral and Octahedral Voids – Radius Ratio – Derivation and its Influence on Structures – **Crystal Structure of Compounds:** Rock Salt – Calcium Chloride – Wurtzite – Zinc Blende – Rutile – Fluorite – Antifluorite – Cadmium Iodide – Nickel Arsenide – Spinel – Normal and Inverse Types – Perovskite Structure – **Theory of Solids:** Free Electron Theory – Band Theory – MO Theory of Solids – **Dislocation in Solids:** Point – Line Defect – Plane Defect – **Superconductors:** BCS Theory – Types of Superconductors – Preparation of HT Superconductors.

UNIT IV – BORON COMPOUNDS AND METAL CLUSTERS

(18 hrs)

Chemistry of Boranes: Nomenclature and Classification of Boranes – Higher Boranes – Preparation, Properties and Structure of Borazines, Boron Nitrides and Hydroborate Ions – Wade's Rule – Styx Number – Carboranes – Types, Preparation, Properties and Structure of Metallocarboranes – Isolobality. A General Study Metal Clusters – **Dinuclear Clusters:** Cu(II) Carboxylate, Chromium(II) Acetate – [Mo₂Cl₈]⁴⁻ and [Re₂Cl₈]⁴⁻ – **Trinuclear Clusters:** [M₃(CO)₁₂] Where M=Fe, Ru, Os – **Tetranuclear Clusters:** [M₄(CO)₁₂] Where M=Co, Rh, Ir. Capping Rule – Polyatomic Zintl Ions – Encapsulation.

UNIT V – INORGANIC POLYMER CHAIN AND CLUSTER COMPOUNDS (18 hrs)

Sulphur - Nitrogen Polymers: Tetrasulphurtetranitride – Disulphurdinitride and Polythiazyl S_xN_y Compounds. **Sulphur-Posphorous Polymers:** P_4S_3 – P_4S_7 – P_4S_9 – P_4S_{10} . **Phosphorous-Nitrogen Polymers:** Phosphazines, Cyclic and Linear Phosphazines. **Silicon Based Polymers:** Silicon Nitrides – Siloxanes. **Isopoly and Heteropoly Acids:** Structure and Bonding of 6- and 12 – Isopoly and Heteropoly Anions . Structure of Silicates - Applications of Paulings Rule of Electrovalence – Isomorphous Replacements in Silicates – Ortho, Meta and Pyro Silicates – One Dimensional – Two Dimensional – Three Dimensional Silicates.

TEXTBOOKS

1. Das A. K. and Das M., *Fundamental concepts of Inorganic Chemistry Vol 1*. CBS Publishers and Distributors, 2015.
2. Das A. K. and Das M. *Fundamental concepts of Inorganic Chemistry Vol 2*. CBS Publishers and Distributors, 2015.,
3. Lee J. D. *Concise Inorganic Chemistry*. Wiley Publication, 5th Edition, 2008.
4. Huheey J.E., Keitler E.A. and Keitler R. L. *Inorganic Chemistry*. New York: Harper Collins College Publishers, 4th Ed., 2012.
5. Atkins P. W., Shriver D. K. and Langford C.H. *Inorganic Chemistry*. U.K: Oxford ELBS, 1990.

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Books

1. Gurdeep Raj. *Advanced Inorganic Chemistry – Vol I*. Meerut: Goel Publishing House, 2015.
2. Cotton F. A. and Wilkinson G. *Advanced Inorganic Chemistry*. Singapore: John Wiley and sons, 5th Ed., 2003.

Web Sources

1. <https://ncert.nic.in/ncerts/l/kech104.pdf>
2. <https://www.youtube.com/watch?v=5AoKAYpr2fs>
3. <https://www.youtube.com/watch?v=ZgVG63c4IzM>

SRI KALISWARI COLLEGE (AUTONOMOUS), SIVAKASI
DEPARTMENT OF CHEMISTRY
PG Programme – M.Sc. Chemistry
SEMESTER - I
CORE COURSE - III: ELECTROCHEMISTRY, THERMODYNAMICS AND
SURFACE CHEMISTRY (21PCHC13)
(From 2021 – 2022 Batch onwards)

HOURS/WEEK: 6
CREDITS : 5
DURATION : 90 hrs

INT. MARKS : 40
EXT. MARKS : 60
MAX. MARKS : 100

Preamble

This course enables the students to gain knowledge in thermodynamics, electro and surface chemistry and spectroscopy.

Course Outcomes (CO)

On successful completion of the course, the learners will be able to

CO1[K2]: explain the various laws of electrochemistry and thermodynamics

CO2[K3]: present the concepts of overvoltage, corrosion, polarography, catalysis and applications of adsorption

CO3[K4]: classify the types of electrodes, catalysis and adsorption

CO4[K5]: deduce the various parameters of thermodynamics and electrochemistry

CO5[K6]: elaborate the concepts and theories of surface and electrochemistry.

CO-PO Mapping table (Course Articulation Matrix)

PO \ CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1 [K2]	3	2	1	1	-	-	-
CO2 [K3]	3	2	1	1	1	1	-
CO3 [K4]	3	2	2	1	1	1	1
CO4 [K5]	3	3	2	1	1	1	1
CO5 [K6]	3	3	2	1	1	1	1
Weightage of the course	15	12	8	5	4	4	3
Weighted percentage of course contribution to POs	5.05	5.02	5.19	4.59	5.19	5.13	4.76

Based on the level of contribution ('3'-High, '2'-Medium, '1'-Low '-' No Correlation)

UNIT I – ELECTROCHEMISTRY - I**(18 hrs)**

Theory of Strong Electrolytes – Inter-Ionic Attraction Theory – Debye-Huckel Theory of Strong Electrolytes – Debye-Huckel Model of Ionic Atmosphere – Debye-Huckel-Onsager Equation – Derivation – Verification and Modifications – Debye-Falkenhagen's Effect – Wien's 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 electrode – Glass Electrode – Platinum Electrode – Glassy Carbon Electrode – Ion Selective Electrode and Measurement of pH.

UNIT II – ELECTROCHEMISTRY - II**(18 hrs)**

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's Rule – Types of Corrosion – Galvanic – Aeration – Stress – Pitting Corrosion – Passivity – Factors Influencing Corrosion – Corrosion Control Method – Cathodic Protection – Corrosion Inhibitors. Principles of Polarography – Cyclic Voltametry – Quasi – Reversible – Irreversible Systems – Basic Principles of Electrochemical Impedance Spectroscopy – Electrochemical Energy Conversions – Nickel-Cadmium Cell – Lead Acid Battery – Fuel Cells – H_2 – O_2 and Methyl Alcohol Fuel Cell – Membrane - Cell Electrode.

UNIT III- THERMODYNAMICS - I**(18 hrs)**

Statement and Mathematical form of First Law of Thermodynamics – Internal Energy – Enthalpy or Heat Content – Heat Capacity - Molar Heat Capacity at Constant Volume (C_v) and at Constant Pressure (C_p) – Relationship Between C_p and C_v – Work Done, Heat Change and Enthalpy Change for Reversible Isothermal Expansion and Compression of an Ideal Gas – Calculation Of Q , W , ΔE , ΔH for Reversible Adiabatic Expansion and Compression of an Ideal Gas – Relation Between T , V and P of an Ideal Gas Undergoing Adiabatic Reversible Expansion of an Ideal Gas – Joule Effect – Joule Thomson Effect - Joule Thomson Coefficient in the case of Ideal and Real Gases – Inversion Temperature.

UNIT IV - THERMODYNAMICS-II**(18 hrs)**

Second Law of Thermodynamics–Statement–Entropy–Definition and Derivation of The Concept of Entropy- Entropy Change in Different Process - Physical Significance (Illustrations With Unavailable Energy, Disorder And Probability)-Work and Gibbs Function- Gibbs-Helmholtz Equations - Variation of Free Energy Change With Temperature and Pressure- Maxwell Relations, Criteria

for Reversible and Irreversible Process. **Partial Molar Properties:** Chemical Potential-Gibbs Duhem Equation-Variation of Chemical Potential With Temperature and Pressure-Claapeyron-Clausius Equation-Concepts of Fugacity and Activity- Determination of Fugacity by Graphical Method-Third Law of Thermodynamics-Statement- Nernst Heat Theorem - Determination of Absolute Entropies of Solids, Liquids and Gases-Test of The Third Law- Exception to the Third Law-Residual Entropy-Calculation of Residual Entropy of CO, NO, N₂O and H₂-Unattainability of Absolute Zero, Entropies of Real Gases, Entropy Change in Chemical Reaction.

UNIT V – SURFACE CHEMISTRY

(18 hrs)

Adsorption: Characteristic of Adsorption – Various Adsorption Isotherm – Freundlich's Adsorption Isotherm – Langmuir Adsorption Isotherm – B.E.T Equation – Determination of Surface Area – Harkins and Jura Method – Benton and White Method – B.E.T. Method – Point B-Method – From Permeability Method – Applications of Adsorption. **Catalysis:** Definition – Types of Catalysis – Characteristics of Catalysis – Theory of Catalysis – Kinetics of Heterogeneous Reactions – Effect of Temperature on Heterogeneous Reactions – Absolute Rate Theory in Heterogeneous Reactions. **Enzyme Catalysis:** Characteristics of Enzyme Catalysis – Factors Affecting the Rate of an Enzyme Reaction – Temperature, pH, Concentration of Substrate – Michaelis and Menten's Equation.

TEXTBOOKS

1. Glasstone Samuel. *An Introduction to Electrochemistry*. Franklin Classes Trade Press, 2018.
2. Kuriacose, Rajaram. *Thermodynamics Classical, Statistical and Irreversible*. Jalandhar: Shobanlal and Co Educational Publishers, 2013.
3. Gurdeep Raj. *Advanced Physical Chemistry*. Jalandhar: GOEL Publication, 2012.

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Books

1. Christine Lefrou, Pierre Fabry and Jean-Claude Poignet. *Electrochemistry: The Basics with Examples*, 2012.
2. Bajpai D. N. *Advanced Physical Chemistry*, New Delhi: S. Chand and Co. Private Limited, 2010.
3. Puri B. R., Sharma L.R. and Pathania M. S. *Text Book of Physical Chemistry*. Jalandhar: Vishal Publishing and Co, 2008.

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1. <https://www.youtube.com/watch?v=KVBw00NSuxg>
2. <https://www.youtube.com/watch?v=x-hQ6oK6HCE>
3. <https://www.youtube.com/watch?v=ReYFJkOhFt4>
4. <https://www.youtube.com/watch?v=jeUW6h2oVEY>
5. <https://www.youtube.com/watch?v=XWaDXanE1WA>

SRI KALISWARI COLLEGE (AUTONOMOUS), SIVAKASI
DEPARTMENT OF CHEMISTRY
PG Programme – M.Sc. Chemistry
SEMESTER - I
CORE COURSE - IV: PRACTICAL: ORGANIC QUANTITATIVE AND
QUALITATIVE ANALYSIS (21PCHC1P)
(From 2021 – 2022 Batch onwards)

HOURS/WEEK: 6
CREDITS : 4
DURATION : 90 hrs

INT. MARKS : 50
EXT. MARKS : 50
MAX. MARKS : 100

Preamble

This course enables the students to gain the practical knowledge in multistep synthesis of organic compounds and quantitative estimation of organic compounds.

Course Outcomes (CO)

On successful completion of the course, the learners will be able to

- CO1[K2]:** explain separation of organic mixture by chemical method
CO2[K3]: perform organic analysis and preparation by following systematic procedure
CO3[K4]: compare the estimation of glucose by different methods
CO4[K5]: decide synthetic route for the preparation of organic compounds by multistep synthesis
CO5[K6]: assemble principles of volumetric analysis for the quantitative estimation of organic compounds.

CO-PO Mapping table (Course Articulation Matrix)

CO \ PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1 [K2]	3	2	1	1	-	-	1
CO2 [K3]	3	2	1	1	-	1	-
CO3 [K4]	3	2	1	1	1	1	-
CO4 [K5]	3	3	2	1	1	1	-
CO5 [K6]	3	3	3	1	2	1	1
Weightage of the course	15	12	8	5	4	4	2
Weighted percentage of Course contribution to POs	5.05	5.02	5.19	4.59	5.19	5.13	3.17

Based on the level of contribution ('3'-High, '2'-Medium, '1'-Low '-' No Correlation)

1. QUANTITATIVE ANALYSIS

1. Estimation of Glucose by Lane and Eynon Method and Bertrand Method
2. Estimation of Glycine
3. Estimation of Formalin
4. Estimation of Methyl Ketone

2. ORGANIC PREPARATION

1. *p*- Nitro Aniline from Acetanilide
2. *p*- Bromoaniline from Acetanilide
3. *m*-Nitrobenzoic Acid from Methyl Benzoate
4. Benzanilide from Benzophenone
5. *Sym*-Tribromobenzene from Aniline

3. QUALITATIVE ANALYSIS OF ORGANIC SALT MIXTURES

Separation and analysis of two component mixture. Identification of the components and preparation of solid derivatives.

REFERENCE

Book

1. Furniss B. S., Hannford A. J., Smith P. W. G. and Tatchell A. R. *Vogel's Textbook of Practical organic chemistry*. England: Longman Scientific and Technical, 5th Ed., 1989.

SRI KALISWARI COLLEGE (AUTONOMOUS), SIVAKASI
DEPARTMENT OF CHEMISTRY
PG Programme – M.Sc. Chemistry
SEMESTER - I
ELECTIVE COURSE - I: GREEN CHEMISTRY (21PCHO11)
(From 2021 – 2022 Batch onwards)

HOURS/WEEK: 6
CREDITS : 4
DURATION : 90 hrs

INT. MARKS : 40
EXT. MARKS : 60
MAX. MARKS : 100

Preamble

This course enables the students to gain knowledge in the field of green chemistry.

Course Outcomes (CO)

On successful completion of the course, the learners will be able to

CO1[K1]: outline the basic principle and methodology involved in the green chemistry

CO2[K2]: explain the ultrasound & microwave assisted and PTC reactions

CO3[K3]: present the concepts of green & sonochemistry, microwave technology and ionic liquids

CO4[K4]: analyse role of green solvents, catalysts and renewable energy involved in the green synthesis

CO5[K5]: predict the synthetic pathway of various organic reactions using greener solvents, catalyst, ionic liquids, biomass and methods

CO-PO Mapping table (Course Articulation Matrix)

CO \ PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1 [K1]	3	2	1	1	-	-	1
CO2 [K2]	3	2	1	1	1	1	-
CO3 [K3]	3	2	2	1	1	1	1
CO4 [K4]	3	3	2	1	1	1	-
CO5 [K5]	3	3	2	1	1	1	1
Weightage of the course	15	12	8	5	4	4	3
Weighted percentage of Course contribution to POs	5.05	5.02	5.19	4.59	5.19	5.13	4.76

Based on the level of contribution ('3'-High, '2'-Medium, '1'-Low '-' No Correlation)

UNIT I - PRINCIPLES AND CONCEPT OF GREEN CHEMISTRY (18 hrs)

Introduction – Concept and Anastas Twelve Principles- Atom Economy Reactions –Rearrangement Reactions-Addition Reactions-Atom Uneconomic-Sublimation-Elimination-Wittig Reactions- Designing a Green Synthesis-Choice of Starting Material-Choice of Reagents-Choice of Catalyst- Choice of Solvents- Green Synthesis of Paracetamol- Nicotinic Acid- Ibuprofen.

UNIT II – SONOCHEMISTRY (18 hrs)

Basic Concepts - Importance of Sonochemistry - Generation of Ultrasound - Magnetostriction Method & Piezoelectric Method - Sonochemical Yield-Ultrasound Assisted Reactions – Esterification, Reduction, Coupling Reactions - Strecker Synthesis, Reformatsky Reaction, Substitution Reaction, Cannizzaro Reaction, Barbier Reaction, Oxidation and Saponification.

UNIT III - MICROWAVE INDUCED GREEN TRANSFORMATIONS (18 hrs)

Design for Energy Efficient Transformations – **Microwave Technology in Chemistry:** Microwave Activation – Theory of Microwave Heating – Advantages of Microwave Heating Over Conventional Heating – Specific Effect of MW - Benefits and Limitations of Organic Synthesis under Microwave. **MW Assisted Reactions in Water:** Hydrolysis – Oxidation Of Toluene And Alcohol – **MW Assisted Reaction in Organic Solvent:** Esterification – Diels – Alder Reaction – *Orthoester* Claisen Rearrangement - **Solvent Free Microwave Assisted Reactions:** Deacetylation – Alkylation of Reactive Methylene Group – Synthesis of Anhydride From Dicarboxylic Acid.

UNIT IV - GREEN SOLVENTS AND CATALYSTS FOR SYNTHESIS (18 hrs)

Water as the Universal Solvent - Introduction- Reaction in Aqueous Phase- Peri Cyclic Reactions- Diel's Alder Reaction-Claisen Rearrangement. **Ionic Liquids:** Types, Preparation and Synthetic Applications – Characteristics and Synthetic Applications - Super Critical CO₂ - Polyethylene Glycol - Green Aspects of Catalysis - Use of Phase Transfer Catalysts for Green Synthesis - Mechanism for PTC Reaction – Advantages of PTC over Conventional Synthesis – Synthetic Applications – Darzen Reaction – Williamson's Ether Synthesis – Wittig Reaction – C – Alkylation – N – Alkylation.

UNIT V- RENEWABLE FEEDSTOCK AND SUSTAINABLE DEVELOPMENT (18 hrs)

Introduction- Biomass: Advantages and Disadvantages Of Biomass as a Chemical Feedstock - Carbohydrate as a Feedstocks for Chemical Production-Lignin as a Renewable Feedstocks - Energy Conversion -Green Chemistry in Education- Industrial Aspects - Bio-Based Renewable-Green Engineering Education for Sustainability for Developing Countries.

TEXTBOOKS

1. Ahulwalia V.K. *New Trends in Green Chemistry*. Anamaya Publishers, New Delhi, Second Edition, 2006.
2. Ahulwalia V.K. and Varma R. S. *Green Solvents for Organic Synthesis*. Narosa Publishing House, New Delhi, 2012.
3. Anastas P. T. *Green Chemistry*. Oxford University Press, New Delhi, Second Edition, 2006.

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1. Anastas P.T. and Williamson T. C. *Green Chemistry- Frontiers in Benign Chemical Synthesis and Processes*. Oxford University Press, 1998.
2. Mike Lancaster. *Green Chemistry An Introductory Text*. RSC publishing, 2nd edition, 2010.

Web Sources

1. <https://www.acs.org/content/acs/en/greenchemistry/principles/12-principles-of-green-chemistry.html>
2. <https://www.youtube.com/watch?v=uLlgbszwlKI>

SRI KALISWARI COLLEGE (AUTONOMOUS), SIVAKASI
DEPARTMENT OF CHEMISTRY
PG Programme – M.Sc. Chemistry
SEMESTER - I
ELECTIVE COURSE - I: MATERIAL CHEMISTRY (21PCHO12)
(From 2021 – 2022 Batch onwards)

HOURS/WEEK: 6
CREDITS : 4
DURATION : 90 hrs

INT. MARKS : 40
EXT. MARKS : 60
MAX. MARKS : 100

Preamble

This course provides the overall ideas on preparation of advanced materials related to nano material, silica based material and polymer based materials.

Course Outcomes (CO)

On successful completion of the course, the learners will be able to

CO1[K1]: recognize the basic knowledge on advanced materials based nanomaterials, silica based material, composite material and polymer materials

CO2[K2]: classify different types of nano materials and polymer materials

CO3[K3]: apply their knowledge in the field of nano chemistry for the preparation of new types of nano materials

CO4[K4]: examine the ways of prediction of advanced materials

CO5[K5]: assess the new types of materials used in the recent research trends.

CO-PO Mapping table (Course Articulation Matrix)

CO \ PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1 [K1]	3	2	1	1	-	-	1
CO2 [K2]	3	2	1	1	1	1	-
CO3 [K3]	3	2	2	1	1	1	1
CO4 [K4]	3	3	2	1	1	1	-
CO5 [K5]	3	3	2	1	1	1	1
Weightage of the course	15	12	8	5	4	4	3
Weighted percentage of Course contribution to POs	5.05	5.02	5.19	4.59	5.19	5.13	4.76

Based on the level of contribution ('3'-High, '2'-Medium, '1'-Low '-' No Correlation)

UNIT I - BASICS OF CRYSTALLINE SOLIDS

(18 hrs)

Crystalline Solids – Crystal Systems – Fundamental of Lattices – Bravais Lattices - Coordination Number – Packing Factors – Cubic – Hexagonal –Diamond Structures – Lattice Planes – Miller Indices – Interplanar Distances – Directions – Types of Bonding – Lattice Energy – Madelung Constants – Born Haber Cycle – Cohesive energy – Symmetry Elements – Operations – Translational Symmetries – Point Groups – Space Groups – Equivalent Positions – Close Packed Structures – Voids – Crystal Structures – Pauling Rules – Defects in crystals – Polymorphism – Twinning.

UNIT II - SILICA BASED MATERIALS (18 hrs)

Introduction to Zeolites – Metallosilicates – Silicalites – Related Microporous Materials – Mesoporous Silica – Metal Oxides – Related Functionalized Mesoporous Materials – Covalent organic Frameworks – Organic – Inorganic Hybrid Materials – Periodic Mesoporous Organo Silica – Metal Organic Frameworks – H₂ /CO₂ Gas Storage and Catalytic Applications.

UNIT III - COMPOSITE MATERIALS (18 hrs)

Introduction - Limitations of Conventional Engineering Materials, Role of Matrix in Composites – Classification - Matrix Materials – Reinforcements - Metal-Matrix Composites – Polymer-Matrix composites – Fibre-Reinforced Composites – Environmental Effects on Composites – Applications of Composites.

UNIT IV - NANO MATERIALS (18 hrs)

Overview of Nanostructures and Nanomaterials: Introduction – Classification – Types of Nano Materials – Nanoparticles – Nanotubes – **Carbon Nanotubes:** Single Walled Carbon Nanotubes and Multi Walled Carbon Nanotubes – Nanowires – Nanoribbons – Nanorods – Nano Composites.**Methods of Preparation:** Top Down Approach – Bottom Up Approach – Chemical Vapour Deposition – Sol-Gel Method – Laser Ablation Method –Electrodeposition Method – Ball Milling Method – Chemical Reduction Method – Spin Coating Technique – Solvothermal Synthesis – Colloidal Method – Co-Precipitation Method – Flame Spray Synthesis (Arc Plasma). **Nanomaterials Characterization:** XRD of Nanomaterials – Electron Microscopy (SEM, TEM, HRTEM and EDX) of Nanomaterials – Scanning Probe Microscopy. **Nanomaterial Properties and Applications:** Magnetic Properties of Nanoparticles – Superparamagnetism – Ferromagnetism in Antiferromagnetic Nanoparticles and Single Domain to Multidomain Transition – Magnetic Nanoparticles as MRI Contrast Agents.

UNIT V - POLYMER SCIENCE AND TECHNOLOGY (18 hrs)

Conducting Polymers: Basic Principles of Conducting Polymers – Delocalized Electronic States of Conjugated Polymers – Polyanilines – Polyacetylenes – Polythiophene – Applications of Conducting Polymers. **Biodegradable Polymers:** Definition Classification of Natural Biodegradable Polymers – Cellulose – Cellulose Acetate – Cellophane – Soy Protein – Corn - Zein Protein - Wheat Gluten Protein – Synthetic Biodegradable Polymers – Polyhydroxyalkanoates – Polycaprolactone – Poly Vinyl Alcohol – Polyacetic Acid – Application of Biodegradable and Biomedical Polymers -Contact Lens, Dental Polymers – Artificial Heart – Kidney – Skin - Blood Cells. **Fibers:** Natural Fibers – Cotton – Wool – Silk – Rayon – Artificial Fibers – Polyamides – Acrylic Acid – PVC – PVA. **Rubber:** Compounding and Elastomeric Properties – Vulcanization – Reinforcement.

TEXTBOOKS

1. Rodger G E. *Inorganic and Solid State Chemistry*. Cengage Learning, 2002.
2. Atkins P, Overton T, Rourke J, Weller M and Armstrong F. *Shriver and Atkins Inorganic Chemistry*, Oxford University Press, 5th Edition, 2012.
3. Poole C. P and Owens, F. J. *Introduction to Nanotechnology*, John Wiley, 2003.
4. Gowariker V. R, Viswanathan N. V, Sreedhar J. *Polymer science*. New Age International Pvt. Ltd, 2015.

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Books

1. Hornyak G. L, Moore J. J, Tibbals H. F, Dutta J. *Fundamental of Nanotechnology*. CRC Press, 2009.
2. Zhen Guo and Li Tan. *Fundamentals and Applications of Nanomaterials*. Artech House London Publication, 2009.
3. Ghosh P., *Polymer Science and technology Plastics, Rubber and composites*. Tata McGraw Hill, 2001.

Web Sources

1. <https://nptel.ac.in/courses/118/104/118104008/>
2. <https://nptel.ac.in/courses/113/104/113104076/>
3. https://onlinecourses.nptel.ac.in/noc20_cy21/preview
4. <https://nptel.ac.in/courses/103/107/103107139/>

SRI KALISWARI COLLEGE (AUTONOMOUS), SIVAKASI
DEPARTMENT OF CHEMISTRY
PG Programme – M.Sc. Chemistry
SEMESTER - I
ELECTIVE COURSE - I: MEDICINAL AND PHARMACEUTICAL CHEMISTRY
(21PCH013)
(From 2021 – 2022 Batch onwards)

HOURS/WEEK: 6
CREDITS : 4
DURATION : 90 hrs

INT. MARKS : 40
EXT. MARKS : 60
MAX. MARKS : 100

Preamble

This course provides the overall ideas on preparation of advanced materials related to nano material, silica based material and polymer based materials.

Course Outcomes (CO)

On successful completion of the course, the learners will be able to

- CO1[K1]:** recognize the various terms used in medicinal and pharmaceutical chemistry
CO2[K2]: express the structural features of various drugs used in pharmaceuticals
CO3[K3]: draw the structure of various drugs used in pharmaceuticals
CO4[K4]: classify the drugs based on their functions and classify the membrane bound receptors
CO5[K5]: appraise the use of various drugs by its action.

CO-PO Mapping table (Course Articulation Matrix)

CO \ PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1 [K1]	3	2	1	1	-	-	1
CO2 [K2]	3	2	1	1	1	1	-
CO3 [K3]	3	2	2	1	1	1	1
CO4 [K4]	3	3	2	1	1	1	-
CO5 [K5]	3	3	2	1	1	1	1
Weightage of the course	15	12	8	5	4	4	3
Weighted percentage of Course contribution to POs	5.05	5.02	5.19	4.59	5.19	5.13	4.76

Based on the level of contribution ('3'-High, '2'-Medium, '1'-Low '-' No Correlation)

UNIT I - FUNDAMENTALS OF MEDICINAL CHEMISTRY (18 hrs)

Definitions of Medicinal Chemistry – Pharmacology and Molecular Pharmacology – 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 Drug (Illustrated With Example).

UNIT II - ANTIBIOTICS, HYPNOTICS AND SEDATIVES (18 hrs)

Antibiotics: Structural Features and Mode of Action of Following Antibiotics – Pencillin G – Cephalosporin and their Semi synthetic Analogs (B-Lactum) – Streptomycin (Aminoglycoside) – Terramycin (Tetracylin) – Erythromycin (Macrolide) and Chloroamphenicol – **Hypnotics and Sedatives:** Introduction – Barbiturates – Phenobarbitones – Amylobarbitone – Pentobarbitone Sodium – Non-Barbiturates – Benzoliazepines – Diazepam – Flurazepam – Flunitrazepam.

UNIT III - ANTINEOPLASTIC AGENTS & ANTITUBERCULARS (18 hrs)

Antineoplastic Agents: Classification – Synthesis – Assay – Cyclophosphamide – Ifosamide – Chlorambucil – Busulfan – Decarbazine – Methotrexate – Azathioprine – 6-Mercaptopurine – 5-Fluorouracil – Cis-platin – **Antitubercular Drugs:** Classification – Synthesis – Assay – Isoniazid – Rifampicin – Pyrazinamine – Ethambutol – Thiacetazone – Para Amino Salicylic Acid and Ethionamide.

UNIT IV - ANTIHYPERTENSIVES AND ANTIHISTAMINES (18 hrs)

Antihypertensive Drugs: Nifedipine – Captopril – Hydralazine - Sodium Nitropruside – Clonidine - Methyldopa and Guanethidine. **Antihistamines:** H₁ – Antagonists: Pheniramine –Chloropheniramine –Diphenhydramine – Mepyramine – Promethazine - H₂ – Antagonists: Cimetidine - Ranitidine and Fomotide.

UNIT V - ANTI-INFLAMMATORY, CNS STIMULANTS AND DEPRESSANTS (18 hrs)

Anti-Inflammatory Drugs: Antipyretics – Non-Narcotic Analgesics – Asprine – Sodium Salicylate – Paracetamol – Phenylbutazone – Oxyphenylbutaxone – Ibuprofen – Mephenamic Acid – Diclofenac Sodium – **CNS Stimulant Drugs:** Amphetamine – Caffeine – Theobromine – Theophylline – Bemegride – Nikethamide – Methyl Phenidate – Peracetum. **CNS Depressant Drugs:** Phenelazine – Isocarboxazide – Amitriptyline - Desipramine.

TEXTBOOKS

1. Chatwal G. R. *Medicinal Chemistry*, Himalaya Publishing House, 2nd Ed., 2002.
2. Jeyashree Ghosh. *A Text Book of Pharmaceutical Chemistry*, New Delhi: S. Chand & Company LTD, 3rd Ed., 2003.

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Books

1. Partrick G. L, *An introduction to Medicinal Chemistry*. II. Oxford University Press, 2001.
2. Nagradi T., *Medicinal Chemistry- A Biochemical Approach*, Oxford University Press, 2004.
3. Taylor J. B. and Kennewell P. D. *Introductory Medicinal Chemistry*, Ellisworth Publishers, 1985.

Web Sources

1. <https://www.youtube.com/watch?v=SEXT6Pulxrc>
2. <https://www.youtube.com/watch?v=eAgwWAlS0io>
3. <https://www.youtube.com/watch?v=9xAod4o2CNA>

SRI KALISWARI COLLEGE (AUTONOMOUS), SIVAKASI

DEPARTMENT OF CHEMISTRY

PG Programme – M.Sc. Chemistry

SEMESTER - II

CORE COURSE - V: REARRANGEMENT, NAME REACTIONS, OXIDATION AND REDUCTION (21PCHC21)

(From 2021 – 2022 Batch onwards)

HOURS/WEEK: 6

CREDITS : 5

DURATION : 90 hrs

INT. MARKS : 40

EXT. MARKS : 60

MAX. MARKS : 100

Preamble

This course enables the students to gain knowledge in addition, elimination and redox reactions.

Course Outcomes (CO)

On successful completion of the course, the learners will be able to

CO1[K2]: interpret the type of reactions to be followed in the selected organic compounds

CO2[K3]: apply the principles of addition, elimination, rearrangement reactions whenever needed

CO3[K4]: compare addition and elimination reactions and reactivity of different oxidizing and reducing reagents

CO4[K5]: deduce the mechanism of given reactions

CO5[K6]: assemble the concept of reaction mechanism and propose scheme for organic reaction.

CO-PO Mapping table (Course Articulation Matrix)

CO \ PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1 [K2]	3	2	1	1	-	-	-
CO2 [K3]	3	2	1	1	1	1	-
CO3 [K4]	3	3	1	1	1	1	-
CO4 [K5]	3	3	2	1	1	1	1
CO5 [K6]	3	3	2	1	1	1	1
Weightage of the course	15	13	7	5	4	4	2
Weighted percentage of course contribution to POs	5.05	5.44	4.55	4.59	5.19	5.13	3.17

Based on the level of contribution ('3'-High, '2'-Medium, '1'-Low '-' No Correlation)

UNIT I - ADDITION TO CARBON-CARBON DOUBLE BOND (18 hrs)

Electrophilic Addition to Carbon – Carbon Double Bonds and Triple Bonds. Nucleophilic Addition to Carbon-Carbon Multiple Bonds – Generation and Addition of Carbenes – Michael Addition and Robinson Annulation – Hydroxylation of Olefinic Double Bonds (OsO_4 , KMnO_4) – Woodward and Prevost Oxidation – Epoxidation using Peracids Including Sharpless Epoxidation – Ozonolysis – Hydrogenation (Homogenous and Heterogeneous) and Transfer Hydrogenation – Hydration of Carbon – Carbon Double and Triple Bonds.

UNIT II - ADDITION TO CARBON-OXYGEN DOUBLE BOND (18 hrs)

Nucleophilic Addition to $>\text{C}=\text{O}$ Bond – Mannich – Benzoin – Darzen's Glycidic Ester – Stobbe – Knoevenagel Condensation Reactions – Wittig-Wittig – Horner Olefination Reactions – Sulfur and Sulfonium Ylides and their Reactions – Julia Olefination & Peterson Alkene Synthesis – Asymmetric Reduction of Carbonyl Functions (Corey's Procedure).

UNIT III - ELIMINATION (18 hrs)

Elimination Reactions $-\text{E}_1$, E_2 , $\text{E}_{1\text{cb}}$ and E_i Eliminations. Conformation of Mechanism – Solvent – Substrate – Leaving Group Effects – Saytzeff's Vs Hoffman Elimination – Stereochemistry of E_2 Eliminations – Elimination in Cyclohexane Ring System – Mechanism of Pyrolytic Eliminations – Examples – Chugaev Reactions and Cope Elimination – Hoffmann Degradation and Pyrolysis of Esters.

UNIT IV - MOLECULAR REARRANGEMENTS & NAME REACTIONS (18 hrs)

A Study of Mechanism of the following Rearrangements – Beckmann – Curtius – Hofmann – Schmidt – Lossen – Wolff – Pinacol – Wagner Meerwin – Demjanov – Dienone-Phenol – Favorski – Benzidine – Claisen – Cope – Sommet – Hauser – Pummerer – Von-Richter Rearrangements. A Study of the following Name Reactions – Dieckmann Cyclization – Hofmann-Löffler Freytag Reaction – Mitsunobu Reaction – Shapiro Reaction – Eschenmoser – Tanabe and Ramburg – Backlund Reactions.

UNIT V - OXIDATION AND REDUCTIONS REACTIONS (18 hrs)

Oxidation with Cr (including PCC, PDC, Jones) and Mn (including MnO_2 and BaMnO_4) Reagents – Oxidation with LTA – DDQ – SeO_2 – Oxidation using Hydroboration – Stereochemistry – Periodic Acid – Osmium Tetraacetate – Lead Tetraacetate – Oppenauer Oxidation – IBX and Dess – Martin Periodinane (DMP) reagent. Reduction with Catalytic Hydrogenation – Metal in liq. Ammonia – Lindlar Catalyst – NaBH_4 – NaCNBH_3 – $\text{Zn}(\text{BH}_4)_2$ LiAlH_4 – $\text{Li}(\text{tBuO})_3\text{AlH}$ – DIBAL-H – Red-Al- Et_3SiH – Bu_3SnH – LDA, 1,3-dithianes – Birch Reduction

TEXTBOOKS

1. Jerry March. *Advanced Organic Chemistry*. John Wiley & Sons, 5th Ed, 2001.
2. Carey F. and Sundberg R. J. *Advanced Organic Chemistry-Part A and B*. Springer Science, 5th Ed, 2007.
3. Smith M. B. and Jerry March. *Advanced Organic Chemistry*. John Wiley & Sons, 5th Ed, 2001.

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Books

1. Clayden J., Greeves N. and Warren S. *Organic Chemistry*. Oxford University Press. 2nd Ed, 2012.
2. Smith M. B. *Organic Synthesis*. Academic Press, 3rd Ed, 2011.
3. Norman R. O. C. and Coxon J. M. *Principles of Organic Synthesis*. Chapman & Hall, 3rd Ed, 1993.

Web Sources

1. <https://nptel.ac.in/content/storage2/courses/104103071/pdf/mod6.pdf>
2. <https://nptel.ac.in/content/storage2/courses/104101005/downloads/LectureNotes/chapter%208.pdf>
3. <https://nptel.ac.in/content/storage2/courses/104101005/downloads/LectureNotes/chapter%2011.pdf>

SRI KALISWARI COLLEGE (AUTONOMOUS), SIVAKASI
DEPARTMENT OF CHEMISTRY
PG Programme – M.Sc. Chemistry
SEMESTER - II
CORE COURSE - VI: COORDINATION, BIOINORGANIC AND INORGANIC
PHOTOCHEMISTRY (21PCHC22)
(From 2021 – 2022 Batch onwards)

HOURS/WEEK: 6
CREDITS : 5
DURATION : 90 hrs

INT. MARKS : 40
EXT. MARKS : 60
MAX. MARKS : 100

Preamble

This course elaborates the theories of bonding, mechanism and photochemistry of complexes and familiarises on the role of metal ions in the biological system, metal toxicology and metals in medicine.

Course Outcomes (CO)

On successful completion of the course, the learners should be able to

- CO1[K1]:** outline on the theories of coordination compounds, biologically important inorganic compound and basics of photochemistry
CO2[K2]: express the various reaction mechanisms involved in coordination compounds and structure of bioinorganic compounds
CO3[K3]: apply the reaction mechanism to synthesize coordination compounds
CO4[K4]: examine the function of bioinorganic compounds and photochemistry of Cr, Co, Cu and Ru complexes
CO5[K5]: deduce the importance of metals in medicine and toxicity.

CO-PO Mapping table (Course Articulation Matrix)

CO \ PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1 [K1]	3	2	1	-	-	-	1
CO2 [K2]	3	2	1	1	1	-	1
CO3 [K3]	3	2	1	1	1	1	-
CO4 [K4]	3	3	2	2	1	1	-
CO5 [K5]	3	3	3	1	1	1	-
Weightage of the course	15	12	8	5	4	3	2
Weighted percentage of Course contribution to POs	5.05	5.02	5.19	4.59	5.19	3.85	3.17

Based on the level of contribution ('3'-High, '2'-Medium, '1'-Low '-' No Correlation)

UNIT I - THEORY OF BONDING IN COORDINATION COMPOUNDS (18 hrs)

Nomenclature of Coordination Complexes - Stereochemistry of Coordination Compounds - Geometrical Isomerism - Optical Isomerism of Complexes having Coordination Number 4 and 6. Complexes - Application of ORD & CD for the Determination of Absolute Configuration of Metal Complexes - Stability of Complexes - Step-Wise and Overall Stability Constant - Factors Affecting Stability Constant in Solution - Determination of Stability Constant by Polarographic and Job's Continuous Variation Method - CFT - Splitting of d - Orbitals in Octahedral - Tetrahedral - Square Planar - Square Pyramid and Trigonal Bipyramidal Geometries - Factors Affecting Crystal Field Splitting - CFSE Calculation in Terms of Δ_o in Octahedral and Tetrahedral Symmetry - Application of CFSE - Spectrochemical Series - Nephelauxetic Effect - MO Theory - Construction of MO Diagram for Sigma and Pi Bonded Octahedral and Tetrahedral Complex.

UNIT II - REACTION MECHANISM OF COORDINATION COMPOUNDS (18 hrs)

Substitution Reactions of Octahedral Complexes - Labile - Inert Complexes - Mechanism - Evidence and Factors Affecting Acid Hydrolysis - Base Hydrolysis and Anation Reactions - Substitution Reactions of Square Planar Complexes - Factors Affecting Reactivity of Square Planar Complexes - The Trans-Effect - Theories and its Applications - Electron Transfer Reactions - Complementary and Non - Complementary Reactions - Outer Sphere and Inner Sphere Electron Transfer Mechanisms - Synthesis of Coordination Complexes Using Electron Transfer and Substitution Reactions.

UNIT III - BIOINORGANIC CHEMISTRY - I (18 hrs)

Metalloporphyrins - Haemoglobin and Myoglobin - Structure and Work Functions - Synthetic Oxygen Carriers - Cytochromes - Structure and Work Functions in Respiration - Chlorophyll - Structure - Photosynthetic Sequence - Iron-Sulphur Protein (Non-Heme Iron Protein) - Copper Containing Proteins - Classification - Blue Copper Proteins - Structure of Blue Copper Electron Transferases - Copper Proteins as Oxidases - Cytochrome C Oxidase - Mechanistic Studies of C Oxidase - Hemocyanin - Copper Enzymes - Azurin - Plastocyanin.

UNIT IV - BIOINORGANIC CHEMISTRY - II (18 hrs)

Metalloenzymes - Carboxy Peptidase A - Structure and Function - Carbonic Anhydrase - Inhibition and Poisoning - Corrin Ring System - Vitamin B₁₂ (Cyanocobalamin) and B₁₂ Co-enzymes - In-Vivo and In-Vitro Nitrogen Fixation - Structure and Function of Biological Membranes - Molecular Mechanism of Ion Transport Across the Membrane - Ionophores - Sodium and Potassium Ion Pumps - Calcium Pump. **Essentials of Trace Elements and Chemical Toxicology:** Trace Elements in Biological System - Metal Ion Toxicity

– Classes of Toxic Metal Compounds – Detoxification. **Metals In Medicine:** Anti-Arthritis Drugs – Au and Cu in Rheumatoid Arthritis – Li in Psychiatry – Pt -Au and Metallocenes in Anti-Cancer Drugs – Metals in Radio diagnosis and Magnetic Resonance Imaging. **Transport and Storage of Metals:** Mechanism – Fe – Cu – Zn and V – Storage and Transport.

UNIT V - PHOTOCHEMISTRY OF TRANSITION METAL COMPLEXES (18 hrs)

Photochemistry of Cr(III) Complexes: Photo-Substitutions – Properties of Ligand Field Excited States – Photo Aquation Reactions – Photolysis Rule – Photoisomerization – Photo Racemisation – Photoanation Reactions – Sensitizer – Energy Transfer Process – Mechanism of Photosensitization – Photo Reactive Excited State – The Doublet Hypothesis – Role of Quartet Excited States – **Photochemistry of Co(III) Complexes:** Introduction – Energy Level Diagram – Photo Aquations in Co(III) Ammine – Co(III) Cyanide Complexes. Fe(II) Low Spin Complexes – Photochemistry of $[\text{Ru}(\text{Bpy})_3]^{2+}$ – Photo Redox Properties of Ce(III) and Ce(IV) Complexes – Photochemistry of Cu(II) (1,3 Diketone) Complexes.

TEXTBOOKS

1. Gopalan and Ramalingam. *Concise Coordination Chemistry*. Vikas Publishing House PVT LTD, 2014
2. G. Whitmore. *Advanced Reaction Mechanism*. New Delhi: IVY Publishing House, 2010.
3. Gurdeep Raj. *Advanced Inorganic Chemistry. Vol I*, Meerut: Goel Publishing House, 2015.
4. Huheey J. E., Keitler E. A and Keitler R. L. *Inorganic Chemistry*. New York: Harper Collins College Publishers, 4thEd., 2012.
5. Atkins P. W., Shriver D. K. and Langford C. H. *Inorganic Chemistry*. U.K: Oxford ELBS, 1990.
6. Lippard S. J. and Berg J.M. *Principle of bioinorganic Chemistry*. University science books, California, 1994.

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1. Cotton F. A. and Wilkinson G. *Advanced Inorganic Chemistry*. Singapore: John Wiley and sons, 5th Ed., 2003.
2. Das A. K. *Inorganic Chemistry Vol-III, Vol-IV Vol-VI*. CBS Publishers and Distributors, 2015
3. Adamson. *Concept of Inorganic Photochemistry*. New York: Wiley, 1975.

Web Sources

1. <https://www.youtube.com/watch?v=6VNXHdM6jis>
2. <https://www.intechopen.com/books/poisoning-in-the-modern-world-new-tricks-for-an-old-dog-/mechanism-and-health-effects-of-heavy-metal-toxicity-in-humans>

SRI KALISWARI COLLEGE (AUTONOMOUS), SIVAKASI
DEPARTMENT OF CHEMISTRY
PG Programme – M.Sc. Chemistry
SEMESTER - II
CORE COURSE - VII: GROUP THEORY, EQUILIBRIA AND STATISTICAL
THERMODYNAMICS (21PCHC23)
(From 2021 – 2022 Batch onwards)

HOURS/WEEK: 6
CREDITS : 5
DURATION : 90 hrs

INT. MARKS : 40
EXT. MARKS : 60
MAX. MARKS : 100

Preamble

This course introduces the learners to group theory, statistical thermodynamics and equilibria.

Course Outcomes (CO)

On successful completion of the course, the learners will be able to

- CO1[K2]:** explain symmetry operations, applications of group theory, concepts of statistical and non- equilibrium thermodynamics
- CO2[K3]:** apply the concepts of group theory and thermodynamics to deduce the point groups and parameters of thermodynamics
- CO4[K3]:** present the theories of phase and chemical equilibria and quantum statistics
- CO5[K4]:** examine the character tables, group multiplication tables, phase diagram for single and double salt.
- CO5[K5]:** predict hybridization and electronic transition of molecules using group theory and theorems of non-equilibrium thermodynamics

CO-PO Mapping table (Course Articulation Matrix)

CO \ PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1 [K2]	3	1	1	1	1	-	-
CO2 [K3]	3	2	1	1	-	-	-
CO3 [K3]	3	3	2	1	1	1	1
CO4 [K4]	3	3	2	1	1	1	-
CO5 [K5]	3	3	2	1	1	1	1
Weightage of the course	15	12	8	5	4	3	2
Weighted percentage of course contribution to POs	5.05	5.02	5.19	4.59	5.19	3.85	3.17

Based on the level of contribution ('3'-High, '2'-Medium, '1'-Low '-' No Correlation)

UNIT I - SYMMETRY IN MOLECULE

(18 hrs)

Symmetry Operations - Symmetry Elements - Rotational Axis of Symmetry - Plane of Symmetry - Improper Rotational Axis - Inversion - Identity. **Properties of a Group:** Closure Rule - Associative Rule - Identity Rule - Inverse Rule - Deducing the Implied Presence of Other Symmetry Elements. **Types of Groups:** Abelian and Non-Abelian groups - Classes and Sub Groups. **Groups Multiplication Table:** C_{2v} , C_{3v} . Point Groups. **Classification of Molecules into Point Groups:** C_{2v} , C_{3v} , C_{2h} , D_{2h} , D_{4h} , D_{6h} , Td and Oh. Vector and Matrix Algebra - Matrix Representation of Symmetry Operations (E, C_n , σ , S_n and i). **Character Table:** Reducible and Irreducible Representations - Great Orthogonality Theorem - Characters - Construction of Character Tables (C_{2v} , C_{3v} , C_{2h} and C_{4v}).

UNIT II - NORMAL MODE OF ANALYSIS

(18 hrs)

Direct Product Concept - Applications of Group Theory to Normal Modes of Vibrations and to Normal Mode Analysis of Water, Ammonia and *Trans* 1,2-Dichloro Ethylene. Spectroscopy Application: Application for Spectral Selection Rules of Vibration Spectra - IR and Raman Active Fundamentals - Symmetry of Molecular Orbitals and Symmetry Selection Rule for Electronic Transitions in Formaldehyde. Group Theory and Quantum Mechanics: Wave Functions as The Basis of Irreducible Representation - Group Theory Applied to Hybridization in Square Pyramidal, BF_3 And $[PtCl_4]^{2-}$ (Character Table Should Be Given). HMO Theory: HMO Calculations and Delocalization Energy for Cyclopropenyl and 1,3-Butadiene Systems.

UNIT III - EQUILIBRIA

(18 hrs)

Phase Equilibria - Three Component System - Formation of One Pair of Partially Miscible Liquids - Formation of Two Pairs of Partially Miscible Liquids - Formation of Three Pair of Partially Miscible Liquids - Two Salt and Water - No Chemical Combination - Double Salt Formed - One Salt Forms a Hydrate. **Chemical equilibria:** Dedonders Concept of Degree of Advancement of a Reaction - Derivation of Law of Mass Action - Experimental Verification of Law of Mass Action - Thermodynamic Derivation of Law of Mass Action - Derivation of Law of Mass Action from Chemical Potential - Van't Hoff Reaction Isotherm - Free Energy Change Method - Le Chatelier's Principle - Applications of Le Chatelier's Principle.

UNIT IV - NON-EQUILIBRIUM THERMODYNAMICS

(18 hrs)

Non-Equilibrium Thermodynamics: Introduction - Postulates of Local Equilibriums - Entropy Production - Forces and Fluxes - Onsager's Reciprocal Relations and Application - Proof of Onsager Reciprocal Relationship - Wiener Theorem - Linear Laws - Stationary States.

Endergonic & Exergonic Reactions: Standard State Free Energy Changes - ΔG , ΔG^0 and $\Delta G'^0$ - Relationship between Equilibrium Constant and $\Delta G'^0$ - Feasibility of Reactions. **ATP:** Structure, Properties and Energy Currency of the Cell - Importance of Coupled Reactions - High Energy Compounds.

UNIT V - STATISTICAL THERMODYNAMICS

(18 hrs)

Definition of State of a System – Ensembles (Micro, Macro and Grand Canonical) - Boltzmann Distribution Law and its Derivation – Boltzmann – Planck Equation – Partition Functions – Translational – Rotational – Vibrational, Electronic Partition Function - Thermodynamics Properties From Partition Functions - Sackur-Tetrode Equation. **Quantum Statistics:** Fermi Dirac and Bose Einstein Statistics – Application of BE Statistics to Photon Gas - Application of FD Statistics to Electron Gas – Einstein's and Debye's Theories of Heat Capacities of Solids.

TEXTBOOKS

1. Cotton F. A. *Chemical Application of Group Theory*. New Delhi: Wiley Eastern Ltd, 2003.
2. Veera Reddy K. *Symmetry and Spectroscopy of Molecules*. Kolkata: New age International Publishers, 2014.
3. Salahuddin Kunju A., Krishnan G. *Group Theory and its Applications in Chemistry*. New Delhi: PHI Learning Private Limited, 2011.
4. Kuriacose, Rajaram. *Thermodynamics Classical, Statistical and Irreversible*. Jalandhar: Shobanlal and Co Educational Publishers, 2013.
5. Gurdeep Raj. *Advanced Physical Chemistry*. Jalandhar: GOEL Publication, 2012.

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1. Ramakrishnan V. and Gopinathan M. S. *Group Theory in Chemistry*. Jalandhar: Vishal Publishing Co, 2000.
2. Bajpai D. N. *Advanced Physical Chemistry*, New Delhi: S. Chand and Co. Private Limited, 2010.
3. Puri B. R., Sharma L.R. and Pathania M. S. *Text Book of Physical Chemistry*. Jalandhar: Vishal Publishing and Co, 2008.

Web Sources

1. <https://www.youtube.com/watch?v=KVBw00NSuxg>
2. <https://www.youtube.com/watch?v=x-hQ6oK6HCE>
3. <https://www.youtube.com/watch?v=ReYFJkOhFt4>
4. <https://www.youtube.com/watch?v=jeUW6h2oVEY>
5. <https://www.youtube.com/watch?v=XWaDXanE1WA>

SRI KALISWARI COLLEGE (AUTONOMOUS), SIVAKASI
DEPARTMENT OF CHEMISTRY
PG Programme – M.Sc. Chemistry
SEMESTER - II
CORE COURSE - VIII: PRACTICAL: INORGANIC QUANTITATIVE AND
QUALITATIVE ANALYSIS (21PCHC2P)
(From 2021 – 2022 Batch onwards)

HOURS/WEEK: 6
CREDITS : 4
DURATION : 90 hrs

INT. MARKS : 50
EXT. MARKS : 50
MAX. MARKS : 100

Preamble

This course develops the skills of the students in the quantitative estimation of metal ions by volumetric, gravimetric and complexometric methods, qualitative analysis of cations in the given inorganic salt mixture and complex preparations

Course Outcomes (CO)

On successful completion of the course, the learners will be able to

- CO1[K2]:** estimate the amount of copper, calcium, ferrous and zinc present in the given solution by volumetrically and the amount of zinc, magnesium, copper and nickel by complexometric titration
- CO2[K3]:** determine the amount of nickel, barium, zinc and copper present in the given solution by gravimetric method
- CO3[K4]:** compare and contrast complexometry, gravimetry & volumetry
- CO4[K5]:** predict the familiar and less familiar cations in the given inorganic salt mixture
- CO5[K6]:** develop the skills and tricks in the inorganic qualitative and quantitative analysis.

CO-PO Mapping table (Course Articulation Matrix)

CO \ PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1 [K2]	3	2	1	1	-	-	-
CO2 [K3]	3	2	1	1	-	1	1
CO3 [K4]	3	2	2	1	1	1	-
CO4 [K5]	3	3	2	1	1	1	1
CO5 [K6]	3	3	2	1	1	1	1
Weightage of the course	15	12	8	5	3	4	3
Weighted percentage of course contribution to POs	5.05	5.02	5.19	4.59	3.9	5.13	4.76

Based on the level of contribution ('3'-High, '2'-Medium, '1'-Low '-' No Correlation)

I. SEMI MICRO QUALITATIVE ANALYSIS

Semi Micro Analysis of Inorganic Mixture Containing Two Familiar Cations and two less Familiar Cations - Maximum of Five Samples.

II. QUANTITATIVE ANALYSIS:

Separation and Estimation of Individual Metal Ion in the Given Mixture by Volumetric and Gravimetric Methods.

- Cu(II) - Volumetric, Ni(II) - Gravimetry
- Cu(II) - Volumetric, Zn(II) - Gravimetry
- Ca(II) - Volumetric, Ba(II) - Gravimetry
- Fe(II) - Volumetric, Ni(II) - Gravimetry
- Fe(II) - Volumetric, Cu(II) - Gravimetry
- Fe(II) - Volumetric, Zn(II) - Gravimetry
- Zn(II) - Volumetric, Cu(II) - Gravimetry

III. INORGANIC PREPARATIONS:

Preparation of at least 8 Inorganic Complexes

IV. 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

REFERENCES

Books

1. Jeffery H., Bassett, Mendham and Denney. *Vogel's Quantitative chemical Analysis*. England: Longman Scientific and Technical, 1989.
2. Ramanujam V. V. *Semimicro Qualitative Analysis*. Madras: The National Publishing Company, 3rd Edn., 1974.

SRI KALISWARI COLLEGE (AUTONOMOUS), SIVAKASI
DEPARTMENT OF CHEMISTRY
PG Programme – M.Sc. Chemistry
SEMESTER - II
NON MAJOR ELECTIVE COURSE: CHEMISTRY FOR HEALTHY LIVING
(21PCHN21)
(From 2021 – 2022 Batch onwards)

HOURS/WEEK: 6
CREDITS : 4
DURATION : 90 hrs

INT. MARKS : 40
EXT. MARKS : 60
MAX. MARKS : 100

Preamble

This course facilitates the students to understand the manufacturing process involved in various chemical industries.

Course Outcomes (CO)

On successful completion of the course, the learners will be able to

CO1[K1]: recognize the technical methods applied in the manufacture of various industrial products

CO2[K2]: explain the raw materials used in chemical industries

CO3[K3]: demonstrate properties and applications of polymers, leather and fuels

CO4[K4]: classify fertilizers, polymers and fuels

CO5[K4]: evaluate the raw materials used in the preparation of rubber industries.

CO-PO Mapping table (Course Articulation Matrix)

PO CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1 [K1]	3	1	-	2	-	2	1
CO2 [K2]	3	1	-	2	-	2	2
CO3 [K3]	2	2	-	2	-	2	1
CO4 [K4]	2	2	1	3	-	-	2
CO5 [K4]	2	1	1	-	-	1	1
Weightage of the course	12	7	2	9	0	7	7
Weighted percentage of Course contribution to POs	4.04	2.93	1.3	8.26	0	8.97	11.11

Based on the level of contribution ('3'-High, '2'-Medium, '1'-Low '-' No Correlation)

UNIT I - RECOMMENDED DIETARY ALLOWANCES & CARBOHYDRATE (18 hrs)

Recommended Dietary Allowances (RDA): Factors Affecting RDA – Principles of Deriving RDA – Requirement and RDA – Balanced Diet – **Carbohydrates:** Classification – Functions – Digestion – Absorption – Maintenance of Blood Glucose Level – Sources.

UNIT II - VEGETABLES AND FRUITS (18 hrs)

Vegetables: Introduction – Classification – Composition and Nutritive Value – Selection – Vegetable Cookery – Storage of Vegetables – Fungi and Algae as Food – **Fruits:** Classification – Composition and Nutritive Value – Post-Harvest Changes and Storage – Enzymatic Browning – Vegetables and Fruits as Functional Foods.

UNIT III - MILK AND MILK PRODUCTS (18 hrs)

Milk and Milk Products: Composition-Physical Properties – Nutritive Value – Effect of Heat – Effect of Acid – Effect of Enzymes – Effect of Phenolic Compounds and Salts – Microorganisms – Milk Products – Milk Substitutes – Role of Milk and Milk Products in Cookery.

UNIT IV - PROTEINS (18 hrs)

Proteins: Introduction-Chemical Composition- Nutritional Classification of Amino Acids – Functions - Specific Functions of Amino Acids - Factors Affecting Protein Utilization-Quality of Proteins – PDCAAS - Complementary Value of Proteins - Recommended Dietary Allowances.

UNIT V - FOOD PRESERVATION (18 hrs)

Food Preservation: Food Spoilage – Methods of Food Preservation – Preservation by Low Temperature – Preservation by High Temperature – Preservation by Preservatives – Preservation by Osmotic Pressure – Preservation by Dehydration – Food Irradiation.

TEXTBOOKS

1. Srilakshmi B. *Nutrition Science*. New Delhi: New Age International Pvt Ltd., 2004.
2. Srilakshmi B. *Food Science*. New Delhi: New Age International Pvt Ltd., 2003.

REFERENCES

Books

1. Snyder C. H. *The Extraordinary Chemistry of Ordinary Things*. New York: John Wiley and Sons Inc., 1992.
2. Krishnamoorthy N., Jeyasubramanian K. and Nayagam P. V. *Applied Chemistry*. New Delhi: Tata McGraw Hill, 1999.

Web Sources

1. <https://nptel.ac.in/courses/104/105/104105040/>
2. <https://www.digimat.in/nptel/courses/video/126105013/L01.html>
3. https://www.youtube.com/watch?v=_Ap4BXhig5c

SRI KALISWARI COLLEGE (AUTONOMOUS), SIVAKASI
DEPARTMENT OF CHEMISTRY
PG Programme – M.Sc. Chemistry
SEMESTER - III
CORE COURSE - IX: SPECTROSCOPY AND SPECTROMETRY (21PCHC31)
(From 2021 – 2022 Batch onwards)

HOURS/WEEK: 6
CREDITS : 5
DURATION : 90 hrs

INT. MARKS : 40
EXT. MARKS : 60
MAX. MARKS : 100

Preamble

This course familiarizes the learners with spectroscopy for the structural elucidation of the organic molecule through UV, IR, NMR and Mass spectra.

Course Outcomes (CO)

On successful completion of the course, the learners will be able to

CO1[K2]: interpret the different functional group, fragments of the molecule through IR and Mass spectra

CO2[K3]: apply the principles of spectroscopy for the structural elucidation of the molecule

CO3[K4]: inspect the structure of organic compounds through different spectroscopic techniques

CO4[K5]: predict the molecular formula of organic compounds by elemental analysis data and structural formula by spectral data

CO5[K6]: elaborate the structure and functional groups present in the organic compound by the application of UV, IR, NMR and Mass spectroscopy.

CO-PO Mapping table (Course Articulation Matrix)

CO \ PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1 [K2]	3	2	1	1	-	1	-
CO2 [K3]	3	2	1	1	1	1	1
CO3 [K4]	3	2	1	1	1	1	-
CO4 [K5]	3	3	2	1	1	1	1
CO5 [K6]	3	3	3	1	1	-	1
Weightage of the course	15	12	8	5	4	4	3
Weighted percentage of course contribution to POs	5.05	5.02	5.19	4.59	5.19	5.13	4.76

Based on the level of contribution ('3'-High, '2'-Medium, '1'-Low '-' No Correlation)

UNIT I - UV AND IR SPECTRA OF ORGANIC COMPOUNDS

(18 hrs)

Electronic Absorption: Beer-Lamberts Law – Types of Electronic Excitation – Chromophore and Auxochrome – Bathochromic – Hypsochromic Shift. **UV-Vis Spectra of Simple Organic Compounds:** Alkenes – Phenols – Anilines – Carbonyl Compounds – 1,3-Diketones – Woodward-Fieser Rule For Conjugated Diene – Dienone Systems. **Infrared Spectra:** Vibrational Frequencies – Fundamental, Overtone and Combination Bands and Factors Affecting Them – Identification of Functional Groups in Organic Compounds – Finger Print Region – Inter and Intramolecular Hydrogen Bonding – Various Factors Affecting IR Stretching Frequencies.

UNIT II - NUCLEAR MAGNETIC RESONANCE & APPLICATIONS

(18 hrs)

Origin of NMR Spectrum – Nuclear Spin States – NMR Active Nuclei – Nuclear Magnetic Moment – Larmor Equation – Absorption of Energy and Resonance – Population Density of Nuclear Spin States – Saturation Phenomena – Relaxation Mechanisms – Comparison of CW and FT Instrument – Chemical Shift – Standards in NMR – Shielding and Deshielding – Factors Affecting Chemical Shift – Electronegativity – Hybridization – Hydrogen Bonding – Anisotropic Effect – Double Bond – Triple Bond – Aromatic Compounds – Carbonyl Compounds and Annulenes – Splitting of Signal-Spin-Spin Coupling – Factors Affecting Coupling Constant – Karplus Equation and Curve – Cis – Trans, Germinal, Vicinal and Long Range Coupling – Ortho – Meta – Para Coupling – Exchange with Deuterium. Dynamic NMR of DMF – Cyclohexane and Iodocyclohexane) – Double Irradiation/Spin Decoupling – Nuclear Overhauser Effect (NOE) and NMR Imaging (MRI).

UNIT III - ^{13}C NMR AND 2-D NMR TECHNIQUES

(18 hrs)

^{13}C NMR: Difficulties in Recording ^{13}C NMR – Homo Nuclear and Hetero Nuclear Coupling – Off Resonance Decoupled Spectrum Identification of Various Types of Carbon (Functional Groups) using ^{13}C NMR – Origin of ^{13}C Satellite Peaks – Attached Proton Test (APT) & Distortionless Enhancement by Polarization Transfer (DEPT) Spectrum (DEPT-45, DEPT-90 and DEPT-135). **Basic Aspects of 2-D NMR Techniques:** Correlation Spectroscopy (COSY) – HOMO COSY (HOMCORR: ^1H - ^1H Connectivity, ^{13}C - ^{13}C Connectivity) – HSQC and HETERO COSY (HETCORR) – HMBC. 2D NOE Correlation Spectroscopy (NOESY).

UNIT IV - MASS SPECTROMETRY

(18 hrs)

Origin, Basics and Bloc Diagram of Mass Spectrum – Various Types of Ionization Techniques – Stability of Molecular Ions, Meta Stable Ions. Base Peaks and Isotope Peaks – Fragmentation Patterns of Organic Molecules – Benzenes – Phenyl Halides – Phenols – Benzyl Alcohols – Benzyl Halides – Aliphatic Alcohols –

Aliphatic as well as Aromatic Aldehydes – Ketones – Acids – Esters - Amides – Aliphatic/Aromatic Nitro Compounds - Amine Compounds (Nitrogen Rule) – Heterocyclic Compounds (Furan, Pyrrole and Pyridine Only) – McLafferty Rearrangements of Organic Molecules.

UNIT V - IDENTIFICATION OF ORGANIC COMPOUNDS USING ANALYTICAL AND SPECTRAL DATA (18 hrs)

Determination of Molecular Formula of Organic Compounds using Elemental (CHN) Analysis Data – Structural Determination of Simple Organic Compounds using UV– IR– NMR and Mass Spectral Data.

TEXTBOOKS

1. Silverstein R.M., Basseler G.C., Morrill T.C. and Bryce D.L. *Spectroscopic Identification of Organic compounds*. John Wiley & Sons, 2015.
2. Jag Mohan. *Organic Spectroscopy, Principle and Applications*. Alpha Science International Ltd, 2004.

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1. Finar I. L. *Organic chemistry Vol II*. Pearson Education, 2001.
2. Clayden J., Greeves N. and Warren S. *Organic Chemistry*. Oxford University Press, 2nd Ed., 2012.

Web Sources

1. https://casegroup.rutgers.edu/lnotes/NMR_lecture.pdf
2. <https://nptel.ac.in/content/storage2/courses/104103071/pdf/mod9.pdf>
3. <https://nptel.ac.in/content/storage2/courses/103108100/module5/module5.pdf>

SRI KALISWARI COLLEGE (AUTONOMOUS), SIVAKASI
DEPARTMENT OF CHEMISTRY
PG Programme – M.Sc. Chemistry
SEMESTER - III
CORE COURSE - X: NUCLEAR, ORGANOMETALICS AND INORGANIC
SPECTROSCOPY (21PCHC32)
(From 2021 – 2022 Batch onwards)

HOURS/WEEK: 6
CREDITS : 5
DURATION : 90 hrs

INT. MARKS : 40
EXT. MARKS : 60
MAX. MARKS : 100

Preamble

This course give in-depth knowledge on various spectroscopy such as electronic spectroscopy, IR, Mossbauer, NMR, ESR, NQR and Photoelectron spectroscopy in the study of inorganic compounds.

Course Outcomes (CO)

On successful completion of the course, the learners will be able to

CO1[K2]: express the principle of the various spectroscopic techniques, organometallics and structure of nucleus

CO2[K2]: explain the structure of inorganic compounds using given spectroscopic data

CO3[K3]: apply the concept of spectroscopy in structural determination of inorganic compounds

CO4[K4]: examine the splitting patterns of Mossbauer, NMR and ESR spectroscopy and structure of metal clusters.

CO5[K5]: evaluate the 10Dq and B values using electronic spectroscopy, spin-orbit coupling using ESR.

CO-PO Mapping table (Course Articulation Matrix)

PO CO	P01	P02	P03	P04	P05	P06	P07
CO1 [K2]	3	2	1	1	-	-	1
CO2 [K2]	3	2	1	1	1	1	-
CO3 [K3]	3	3	1	1	1	1	1
CO4 [K4]	3	3	2	1	1	1	-
CO5 [K5]	3	3	3	1	1	1	-
Weightage of the course	15	13	8	5	4	4	2
Weighted percentage of Course contribution to POs	5.05	5.44	5.19	4.59	5.19	5.13	3.17

Based on the level of contribution ('3'-High, '2'-Medium, '1'-Low '-' No Correlation)

UNIT I

(18 hrs)

Structure of Nucleus and Radioactivity Decay: Composition of The Nucleus – Nuclear Size, Shape and Density – Principal, Radial and Magnetic Quantum Numbers – Magnetic and Electric Property of Nucleus – Elementary Treatment of Shell (Independent Particle) Model – Nuclear Configuration – Parity and Its Conservation – Mass Defect and Binding Energy – Nuclear Forces Theory. **Radioactive Decay:** Group Displacement Law – Decay Series – Rate of Disintegration – Half Life – Average Life – Units of Radioactivity – Secular and Transient Equilibria – Nuclear Isomerism – Internal Conversion and Electron Capture.

UNIT II

(18 hrs)

Organometallic Chemistry and Metal Clusters: Concept of Hapticity of Organic Ligands - **Metal Carbonyls:** 18 Electron Rule, Electron Count of Mononuclear - Polynuclear and Substituted Metal Carbonyls of 3d Series. Structures of Mononuclear and Binuclear Carbonyls of Cr, Mn, Fe, Co and Ni Using VBT. **π -Acceptor Behaviour of CO(MO Diagram of CO to be Discussed):** Synergic Effect and Use of IR Data to Explain Extent of Back Bonding - **Metal Alkyls:** Important Structural Features of Methylaluminum (Tetramer) and Trialkylaluminum (Dimer) - concept of Multicentre Bonding in these Compounds - Role of Triethylaluminum in Polymerisation of Ethane - **Bonding and Structure of Following Clusters:** Dinuclear Clusters: Cu(II)Carboxylate, Chromium(II)Acetate - $[\text{Mo}_2\text{Cl}_8]^{4-}$ and $[\text{Re}_2\text{Cl}_8]^{4-}$ Trinuclear Clusters: $[\text{M}_3(\text{CO})_{12}]$ Where M=Fe, Ru, Os - Tetranuclear Clusters: $[\text{M}_4(\text{CO})_{12}]$ Where M= Co, Rh, Ir - Capping Rule- Polyatomic Zintl Ions - Encapsulation.

UNIT III - ELECTRONIC SPECTRA OF TRANSITION METAL COMPLEXES (18 hrs)

Types of Transition - d-d Transition – Charge Transfer Transition – Atomic and molecular term symbols – Selection Rules – Mechanism of Breakdown of Selection Rules – Bandwidths and Shapes – Jahn-Teller Effect - Orgel Diagram for d^n System – Tanabe-Sugano Diagram – Evaluation of $10Dq$ and B for Octahedral and Tetrahedral Complexes of d^3 and d^8 Configurations.

UNIT IV - IR AND MOSSBAUER SPECTROSCOPY

(18hrs)

Application of IR Spectra in the Study of Coordination Compounds: Application to Metal Carbonyls – Nitrosyls – Carbonate - H_2O , -OH, -CN, -SCN, -NO₂ – Geometrical and Linkage Isomerism. Stretching Mode Analysis of Metal Carbonyls. **Mossbauer Spectroscopy:** Mossbauer Effect - Resonance Absorption – Doppler Effect – Doppler Velocity – Experimental Technique of Measuring Resonance Absorption – Isomer Shift – Quadrupole Splitting - Magnetic Hyperfine Splitting – Application of Mossbauer Spectroscopy in the Study of Iron and Tin Complexes.

UNIT V - NMR and EPR Spectroscopy

(18hrs)

NMR Spectroscopy: Introduction – ^{31}P , ^{19}F and ^{15}N – NMR – Introduction – Application in Structural Problem of the Compounds Like ClF_3 - SF_6 - PF_5 - BrF_5 - H_2PF_3 - $\text{PF}_3(\text{NH}_2)_2$ - PCl_5 - Various acids of Phosphorous - P_4S_3 - Cis and Trans HCONH_2 - $\text{PtCl}_2(\text{PBU}_3)(\text{PPh}_3)_3$ - $\text{P}_3\text{N}_3\text{Cl}_4\text{F}_2$ - $\text{P}_4\text{N}_4\text{Cl}_6(\text{NHC}_6\text{H}_5)_2$ – Dynamic NMR-NMR of Fluxional Molecules – Contact Shift and Shift Reagents.

EPR: Principles – Presentation of the Spectrum – Hyperfine Splitting – Evaluation of g and A Tensors Factor Affecting the Magnitude of g Values - Zero Field Splitting – Kramer's Degeneracy – Anisotropy and Hyperfine Splitting Constant - ESR in the Study of Transition Metal ESR Spectra of V(II) - Mn(II) Fe (II) - Co (II) - Ni(II) - Cu (II) Complexes - Bis(Salicylaldimine) Copper(II) - $[(\text{NH}_3)_5\text{Co}-\text{O}_2-\text{Co}(\text{NH}_3)_5]$ and Mn^{2+} Complexes– John Teller Distortion Studies in Cu (II) Complexes- Evaluation of Spin-Orbit Coupling.

TEXTBOOKS

1. Atkins P. W., Shriver D. K. and Langford C. H. *Inorganic Chemistry*. U. K: Oxford ELBS, 1990.
2. Drago R. S. *Physical Methods in Chemistry*, London: Saunders Golden Sunburst Series, W.B. Saunders Company, 1997.
3. James E. Huheey, Ellen A. Keitler and Richard L. Keitler. *Inorganic Chemistry*. New York: Harper Collins College Publishers, 4th Edition, 2012.
4. Gopalan and Ramalingam. *Concise Coordination Chemistry*, Vikas Publishing House PVT LTD, 2014.

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1. Kettle S. F. A. *Coordination Chemistry*. Spectrum Academic Publishers Oxford, 1996.
2. Asim K. Das. *Inorganic Chemistry. Vol II, V and VIII*. CBS Publishers and Distributors, 2015.

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1. <https://www.dalalinstitute.com/books/a-textbook-of-inorganic-chemistry-volume-1/electronic-spectra-of-transition-metal-complexes/>
2. <http://edujournal.in/nmrnqrepr-and-mossbauer-in-inorganic-chemistry-download-free-pdf/>
3. <https://store.kortext.com/nmr-spectroscopy-in-inorganic-chemistry-633446>
4. [https://chem.libretexts.org/Bookshelves/Inorganic_Chemistry/Map%3A_Inorganic_Chemistry_\(Housecroft\)/04%3A_Experimental_techniques/4.12%3A_A_Photoelectron_Spectroscopy_\(PES_UPS_XPS_ESCA\)](https://chem.libretexts.org/Bookshelves/Inorganic_Chemistry/Map%3A_Inorganic_Chemistry_(Housecroft)/04%3A_Experimental_techniques/4.12%3A_A_Photoelectron_Spectroscopy_(PES_UPS_XPS_ESCA))
5. <https://www.kobo.com/us/en/ebook/photoelectron-spectroscopy>

SRI KALISWARI COLLEGE (AUTONOMOUS), SIVAKASI
DEPARTMENT OF CHEMISTRY

PG Programme – M.Sc. Chemistry

SEMESTER - III

CORE COURSE - XI: SPECTROSCOPY AND PHOTOCHEMISTRY (21PCHC33)
(From 2021 – 2022 Batch onwards)

HOURS/WEEK: 6

CREDITS : 5

DURATION : 90 hrs

INT. MARKS : 40

EXT. MARKS : 60

MAX. MARKS : 100

Preamble

This course enables the students to gain knowledge in electrochemistry and spectroscopy.

Course Outcomes (CO)

On successful completion of the course, the learners will be able to

CO1[K2]: express the basic principle involved in the spectroscopy and photochemistry

CO2[K3]: apply the principle of spectroscopy to identify the rotational, Vibrational and electronic translational involved in the molecules

CO3[K4]: analyse the possible electronic transitions by applying selection rules and width and intensity of spectral lines and techniques in the photochemistry

CO4[K5]: predict the structure of known and unknown compounds by various spectroscopic techniques.

CO5[K6]: elaborate the various types of spectra and physical properties of excited state of molecules

CO-PO Mapping table (Course Articulation Matrix)

CO \ PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1 [K2]	3	2	1	1	1	-	-
CO2 [K3]	3	2	1	1	-	1	-
CO3 [K4]	3	2	2	1	-	1	1
CO4 [K5]	3	3	2	1	1	1	-
CO5 [K6]	3	3	2	1	2	1	1
Weightage of the course	15	12	8	5	4	4	2
Weighted percentage of Course contribution to POs	5.05	5.02	5.19	4.59	5.19	5.13	3.17

Based on the level of contribution ('3'-High, '2'-Medium, '1'-Low '-' No Correlation)

UNIT I – SPECTROSCOPY - I

(18 hrs)

Electromagnetic Spectrum: Region of the Spectrum – Absorption and Emission of Radiation – Einstein's Coefficient – Width of Spectral Line – Intensity of Spectral Line. **Rotational Spectroscopy:** Classification of Molecules by Moments of Inertia - Rotational Spectra of Rigid Diatomic Molecules – Intensities of Spectral Line – Effect of Isotopic Substitution – Rotational Spectra of Polyatomic Linear Molecule – Chemical Analysis by Rotational Spectra. **Infrared Spectroscopy:** Vibrational Energy of a Diatomic Molecule – The Simple Harmonic Oscillator – The Anharmonic Oscillator – Infrared Selection Rules – Diatomic Vibrating Rotator – Interaction of Rotation and Vibration – Vibrations of Polyatomic Molecules – Overtone, Combination and Difference Bands – Coupling Interaction – Fermi Resonance – Fourier Transform Infrared Spectroscopy.

UNIT II – SPECTROSCOPY - II

(18 hrs)

Raman Spectroscopy: Theories of Raman Scattering. **Pure Rotational Raman Spectra:** Linear Molecule – Symmetric Top Molecule. **Vibrational Raman Spectra:** Raman Activity of Vibration – Mutual Exclusion – Rotational Fine Structure – Principle of Laser Raman Spectra. **Electronic Spectroscopy:** Electronic Spectra 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 Pre-dissociation Spectra. **NQR:** Principles and Applications – Quadrupole Moment and Electrical Field – Nuclear Quadrupole Resonance – Nuclear Quadrupole Coupling in Atoms and Molecules – Identification of Ionic Character and Hybridization.

UNIT III – SPECTROSCOPY - III

(18 hrs)

NMR: Magnetic Properties of Nuclei – Resonance – Condition – NMR Instrumentation – Relaxation Processes – Bloch Equations – Chemical Shift – Spin-Spin Coupling – Relaxation Times – Line Shape and Line Width Experimental Technique – Double Resonance Technique – ENDOR – Overhauser Effect – FT-NMR Spectroscopy – Lanthanide Shift Reagents – NMR Imaging. **ESR:** Principles of ESR – g Factor – Hyperfine Structure – Fine Structure – Double Resonance in ESR – Techniques of ESR Spectroscopy – ESR Spectra of Hydrogen Atom – Methyl Radical – 1,4-Benzosemiquinone Radical Anion – Naphthalene Negative Ion – Anthracene Negative Ion – Triphenylmethyl Radical. **ESR of Anisotropic Systems:** Zero Field Splitting and Kramer's Degeneracy in ESR – Multi Resonance Techniques in ESR Spectroscopy.

UNIT IV–PHOTO PHYSICAL PROCESS

(18 hrs)

Types of Photophysical Pathways - Radiation Less Transition - Internal Conversion and Intersystem Crossing - Fluorescence Emission - Fluorescence and Structure - Triplet States and Phosphorescence Emission-Emission Property and the Electronic Configuration - Photophysical Kinetics of Unimolecular Processes - Diagram-Delayed Fluorescence - The Effect of Temperature on Emission Process. Classification of Photochemical Reactions - Rate Constants and Lifetimes of Reactive Energy State-Effect of Light Intensity on the Rate of Photochemical Reactions - Types of Photochemical Reactions - Reaction between Hydrogen and Bromine - Reaction between Hydrogen and Iodine.

UNIT V – PHYSICAL PROPERTIES OF EXCITED MOLECULE

(18 hrs)

Nature of Changes on Electronic Excitation – Electronic, Vibrational and Rotational Energies-Potential Energy Diagram-Shapes of Absorption Band - Franck-Condon Principle - Emission Spectra - Environmental Effect on Absorption and Emission Spectra - Excited State Dipole Moment-Excited State Acidity Constant - Excited State Redox Potential - Emission of Polarized Luminescence - Geometry of some Electronically Excited Molecule - Wigner's Spin Conservation. **Tools And Techniques In Photochemistry:** Origin of Life - Mutagenic Effect of Radiation – Photosynthesis - Photo Electrochemistry of Excited State Redox Reaction - Solar Energy Conversion and Storage - Light Source - Measurement of Emission – Techniques for Study of Transient Species in Photochemical Reactions - Laser in Photochemical Kinetics.

TEXTBOOKS

1. Banwell C. N. *Fundamentals of Molecular Spectroscopy*. New Delhi: Tata McGraw Hill Education Private Limited, 2011.
2. Aruldas G. *Molecular Structure and Spectroscopy*. Eastern Economy Edition, 2nd Edition, 2008.
3. Rohatgi Mukherjee K. K. *Fundamentals of Photo Chemistry*. Jalandhar: New Age International Publishers, 2003.

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Books

1. Peter Atkins and Julio de Paula, *Atkins Physical Chemistry*. Oxford Press, 10th edition.
2. Puri, Sharma, Pathania. *Principles of Physical Chemistry*. Jalandhar: Vishal Publishing Co, 2016.
3. Bajpai D. N. *Advanced Physical Chemistry*, New Delhi: S. Chand and Co. Private Limited, 2010.

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1. https://www.youtube.com/watch?v=l2ENx_Y0dNU
2. <https://www.youtube.com/watch?v=4j5cMHVPStc>
3. <https://www.youtube.com/watch?v=4j5cMHVPStc>
4. <https://www.youtube.com/watch?v=TXW0T3RhBRE>

SRI KALISWARI COLLEGE (AUTONOMOUS), SIVAKASI
DEPARTMENT OF CHEMISTRY
PG Programme – M.Sc. Chemistry
SEMESTER - III
CORE COURSE - XII: PRACTICAL: PHYSICAL CHEMISTRY (21PCHC3P)
(From 2021 – 2022 Batch onwards)

HOURS/WEEK: 6
CREDITS : 4
DURATION : 90 hrs

INT. MARKS : 50
EXT. MARKS : 50
MAX. MARKS : 100

Preamble

This course enables the students to acquire the practical knowledge in electrochemistry and surface chemistry.

Course Outcomes (CO)

On successful completion of the course, the learners will be able to

- CO1[K2]:** demonstrate adsorption, conductometric titration and potentiometric titration
- CO2[K3]:** perform the precipitation titrations, potentiometric redox titrations and adsorption experiments
- CO3[K3]:** apply the principle of conductometry and potentiometry to carry out precipitation and redox titration
- CO4[K4]:** examine the strength of acid by adsorption experiments
- CO5[K5]:** evaluate solubility product by potentiometric method and dissociation constant by conductometric methods.

CO-PO Mapping table (Course Articulation Matrix)

CO \ PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1 [K2]	3	2	1	1	-	-	1
CO2 [K3]	3	2	1	1	1	1	1
CO3 [K3]	3	3	2	1	1	1	1
CO4 [K4]	3	3	2	1	1	1	-
CO5 [K5]	3	3	2	1	1	1	-
Weightage of the course	15	13	8	5	4	4	3
Weighted percentage of course contribution to POs	5.05	5.44	5.19	4.59	5.19	5.13	4.76

Based on the level of contribution ('3'-High, '2'-Medium, '1'-Low '-' No Correlation)

I. CONDUCTOMETRIC EXPERIMENTS

- (i) Double Displacement and Acid Base Titrations
 - (a) Estimation of Mixture of Acids (CH_3COOH & HCl)
 - (b) Estimation of Mixture of Acids (NH_4Cl & HCl)
- (ii) Determination of Solubility Product of Sparingly Soluble Salts
- (iii) Precipitation Titration
 - Estimation of Na_2CO_3
 - Estimation of BaCl_2
- (iv) Determination of Dissociation Constant of Acetic acid.

II. POTENTIOMETRIC METHODS

- (i) Redox Titrations
 - Estimation of Fe(II) Using CAS
 - Estimation of KI with KMnO_4
 - Estimation of Fe(II) Using $\text{K}_2\text{Cr}_2\text{O}_7$
- (ii) Determination of Solubility Product of Sparingly Soluble Salts.
- (iii) Determination of pH of Buffer Solutions.
- (iv) Determination of Dissociation Constant of Weak Acids.

III. ADSORPTION EXPERIMENTS

- Adsorption of Oxalic Acid on Activated Charcoal.
- Adsorption of Acetic Acid on Activated Charcoal.

III. KINETIC EXPERIMENTS

- (i) Kinetics of Acid Hydrolysis an Ester and Compare the Strengths of Acids.
- (ii) Study of Primary Salt Effect and Determination of the Concentration of Given KNO_3 .

REFERENCES

Books

1. Thomas A. O. *Practical Chemistry*. Kerala: Scientific Book Centre, 1999.
2. Gupta and Renu. *Practical Physical Chemistry*. Kerala: New Age International (P) Ltd Publishers, 2017.

SRI KALISWARI COLLEGE (AUTONOMOUS), SIVAKASI
DEPARTMENT OF CHEMISTRY
PG Programme – M.Sc. Chemistry
SEMESTER - III
ELECTIVE COURSE - II: NUCLEAR REACTIONS, RADIATION CHEMISTRY,
PHOTOELECTRON SPECTROSCOPY AND ORGANOMETALLICS IN INDUSTRY
(21PCH031)
(From 2021 – 2022 Batch onwards)

HOURS/WEEK: 6
CREDITS : 4
DURATION : 90 hrs

INT. MARKS : 40
EXT. MARKS : 60
MAX. MARKS : 100

Preamble

This course elaborates the various concepts in nuclear and radiation chemistry with their applications.

Course Outcomes (CO)

On successful completion of the course, the learners will be able to

CO1[K2]: express the basic concepts of nuclear reactions, radiation, NQR, PES and magnetic behavior of complexes.

CO2[K3]: apply concepts of nuclear and radiation chemistry in various fields

CO3[K4]: compare

CO4[K5]: measure the radioactivity by various techniques and examine the use of tracer isotopes in various fields

CO5[K5]: appraise the applications of radioactive isotopes, NQR, PES and AES.

CO-PO Mapping table (Course Articulation Matrix)

CO \ PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1 [K2]	3	2	1	1	-	-	-
CO2 [K3]	3	2	1	1	1	1	1
CO3 [K4]	3	2	2	1	1	1	-
CO4 [K5]	3	3	2	1	1	-	1
CO5 [K5]	3	3	2	2	1	1	-
Weightage of the course	15	12	8	6	4	3	2
Weighted percentage of Course contribution to POs	5.05	5.02	5.19	5.5	5.19	3.85	3.17

Based on the level of contribution ('3'-High, '2'-Medium, '1'-Low '-' No Correlation)

UNIT I – NUCLEAR REACTIONS AND APPLICATION

(18 hrs)

Bethe's Notation of Nuclear Process – Types of Nuclear Reactions - Nuclear Reaction Energies (Q Value) – Compound Nucleus Theory - Nuclear Fission – Energy Release in Nuclear Fission – Mass Distribution of Fission Products – Theory of Nuclear Fission– Fissile and Fertile Isotopes – Energy from Nuclear Fusion - Thermonuclear Reactions in Stars – Power Nuclear Reactor – Breeder Reactor – Nuclear Reactors in India – **Application of Radioactive Isotopes:** Characteristics of Reprocessing of Spent Fuels: Recovery of Uranium and Plutonium - Tracer Isotopes – Chemical Investigation – Age Determination – Medical Field – Agriculture – Industry – Analytical Application – Isotope Dilution Analysis – Neutron Activation Analysis – Biological Effects of Radiation – Waste Disposal Management

UNIT II – RADIATION CHEMISTRY

(18 hrs)

Elementary Ideas of Radiation Chemistry – Interaction of Radiation with Matters – Radiation Dosimetry - Units of Radiation Energy (Rad, Gray, Rontgen, RBE, RCM, Sievert) – Radiation Dosimeter - Fricke's Dosimeter - Ceric Sulphate Dosimeter - Radiolysis of Water and Aqueous Solutions - Unit of Radiation Chemical Yield (G-Value) – Radiation Induced Color Centers in Crystals. Measurement of Radioactivity - Idea about Accelerator and Detectors - Van De Graaf and Linear Accelerators – Synchrotrons - Geiger-Muller Detector -Scintillation Detectors – Applications: Radiometric Titration – Prospecting of Natural Resources

UNIT III - NQR AND PHOTOELECTRON SPECTROSCOPY

(18 hrs)

NQR: Principles – Quadrupole Moment - Electric Field Gradient - Nuclear Quadrupole Resonance - Nuclear Quadrupole Coupling in Atoms and Molecules – Applications to Inorganic Molecules - Identification of Ionic Character and Hybridization. **Photoelectron Spectroscopy:** Theory – XPS – UV – PES – Instrumentation - Evaluation of Ionization Potential – Chemical Identification of Elements – Koopmann's Theorem – Chemical Shift – UPS – XPES of N₂, O₂ and HCl – Evaluation of Vibrational Constants from UPS – Spin – Orbit Coupling. **Auger Spectroscopy:** Principle and its Application.

UNIT IV - MAGNETIC BEHAVIOUR AND PI-COMPLEXES

(18 hrs)

Types of Magnetic Behaviour in Coordination: Types of Magnetism - Magnetic Properties of Free Ions - Temperature Dependence of Magnetism (TDP) - Temperature Independent Paramagnetism (TIP) - Spin State Crossover, Antiferromagnetism - Inter and Intra Molecular Interaction. Application of Magnetic Measurements in the Determination of Structure of Transition Metal Complexes - **Pi-Complexes:** Pi Complexes With Sigma Base, Pi Acid Ligands - EAN Rule - Isolobal

Relationship - Structure and Bonding of Metal Carbonyls - Metal Nitrosyls - Molecular Oxygen Complexes

.UNIT V – ORGANOMETALLIC CHEMISTRY

(18 hrs)

Application of Organometallic Compound in Industry: Synthesis – Properties - Structure and Bonding in Ferrocene – Arene – Olefin - Acetylene and Allyl Complexes - **Catalysis Using Organometallic Compounds:** Oxidative Addition – Reductive Elimination – Insertion Reaction – **Catalytic Mechanism in the Following Reactions:** Hydrogenation Of Olefins (Wilkinson Catalyst) – Tolman Catalytic Loops – Hydroformylation (Oxo Process) – Acetic Acid from Ethanol – Oxidation of Alkenes to Aldehydes and Ketone (Wacker Process) Catalysis in the Formation of Synthesis Gas - Homologation- Water Gas Shift Reaction-Synthetic Gasoline (Fischer-Tropsch and Mobil Process) – Olefin Polymerization (Ziegler – Natta) – Cyclo Oligomerisation of Acetylenes (Reppe's or Wilke's Catalysts) – Olefin Isomerisation Using Ni Catalyst.

TEXTBOOKS

1. Arnikaar H. J. *Essentials of Nuclear Chemistry*. New Delhi: Wiley Eastern, New age international (P) Limited Publishers, 4th Ed., 1997.
2. Soni P.L. and Mohan Katyal. *Textbook of Inorganic Chemistry - A Modern approach*. New Delhi: Sultan Chand and Sons, 2003.
3. Puri B. R., Sharma L. R. and Kalia K. C. *Principles of Inorganic Chemistry*, Delhi: Mile stone publishers and distributor, 31st Edition, 2013.

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Books

1. Glasstone S. *Source Book on Atomic Energy*, New York: Van Nostrand Reinhold Company, 1967.
2. Friedlander G., Kennedy J. W., Macias E. S. and Miller J.M. *Nuclear and Radiochemistry*. New York: John Wiley and Sons Inc., 1981.
3. Dash U. N. *Nuclear Chemistry*, New Delhi: Sultan Chand and sons, 1991.
4. Nesmeyanov A. N. *Radiochemistry*, Moscow: MIR Publication, 1974.
5. Spinks J. W. T. and Woods R. J. *An Introduction to Radiation Chemistry*. New York: John-Wiley and Sons, 3rd Ed., 1990.

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1. <https://www.elsevier.com/books/radiochemistry-and-nuclear-chemistry/choppin/978-0-7506-2300-1>
2. <https://onlinelibrary.wiley.com/doi/book/10.1002/9783527653331>
3. <https://www.elsevier.com/books/radiochemistry-and-nuclear-chemistry/choppin/978-0-7506-7463-8>

SRI KALISWARI COLLEGE (AUTONOMOUS), SIVAKASI

DEPARTMENT OF CHEMISTRY

PG Programme – M.Sc. Chemistry

SEMESTER - III

ELECTIVE COURSE - II: ADVANCED ANALYTICAL CHEMISTRY (21PCH032)

(From 2021 – 2022 Batch onwards)

HOURS/WEEK: 6

CREDITS : 4

DURATION : 90 hrs

INT. MARKS : 40

EXT. MARKS : 60

MAX. MARKS : 100

Preamble

The learners should be able to apply the conceptual understanding of the principles and applications of analytical techniques.

Course Outcomes (CO)

On successful completion of the course, the learners will be able to

CO1[K2]: explain the principles applications of instrumentation techniques

CO2[K3]: apply statistical procedure to carry out data analysis

CO3[K4]: examine analytes by electro analytical, chromatographic and spectroscopic techniques

CO4[K5]: assess electroanalytical techniques and spectroscopic techniques for chemical analysis.

CO5[K5]: select suitable physical methods of characterization

CO-PO Mapping table (Course Articulation Matrix)

PO \ CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1 [K2]	3	2	1	1	-	-	-
CO2 [K3]	3	2	1	1	1	1	1
CO3 [K4]	3	2	2	1	1	1	-
CO4 [K5]	3	3	2	1	1	-	1
CO5 [K5]	3	3	2	2	1	1	-
Weightage of the course	15	12	8	6	4	3	2
Weighted percentage of Course contribution to POs	5.05	5.02	5.19	5.5	5.19	3.85	3.17

Based on the level of contribution ('3'-High, '2'-Medium, '1'-Low '-' No Correlation)

UNIT I - STATISTICAL FOR ANALYTICAL EXPERIMENTATION (18 hrs)
Probability - Regression Analysis - Accuracy and Propagation of Errors - Data Analysis - Signal Enhancement.

UNIT II - ADVANCED CHROMATOGRAPHIC TECHNIQUES (18 hrs)
Theory of Separation Methods: HPLC – GC - GC/MC - LC/MC – GPC - Detectors in Chromatography - Applications of Chromatography.

UNIT III - ELECTROANALYTICAL TECHNIQUES (18 hrs)
Principles of Potentiometry – Electrogravimetry – Voltametry - Stripping methods - Quantitative Applications of Potentiometry and Voltametry - Electrochemical Sensors.

UNIT IV - SPECTROMETRIC AND SPECTROSCOPIC METHODS (18 hrs)
Methodology in Spectrochemical Analysis - Spectrophotometry – Introduction to Electromagnetic Radiation - Optical Components of a Spectrometer – Sources – Detectors. Atomic Adsorption and Emission Spectroscopy - Principles and Applications of Fluorimetry.

UNIT V - PHYSICAL METHODS OF CHARACTERIZATION (18 hrs)
Surface Techniques - Principles and Applications of Electron Spectroscopy for Chemical Analysis and Scanning Probe Microscopy.

TEXTBOOKS

1. Mendham J., *Vogel's A. I. Quantitative Chemical Analysis*. Pearson. 6th Ed., 2009.
2. Day R. A., Underwood A. L. *Quantitative Chemical Analysis*. PHI Learning PVT, Ltd, 6th Ed., 2001.

REFERENCES

Books

1. Skoog D. A., West D. M, Holler F. J. and Grouch S. R. *Fundamental of Analytical Chemistry*. Sounders College Publishers, 8th Ed., 2007.
2. Jeffery G. H., Bassett J., Mendham J. and Denny R. C. *Vogel's Text book of Quantitative Chemical Analysis*. John Wiley & Sons, 5th Ed., 1989.

Web Sources

1. <https://youtu.be/NLJDt88BPMg>
2. <https://youtu.be/SCEZoFmiUuk>
3. <https://youtu.be/SFJ0HXRz-o4>

SRI KALISWARI COLLEGE (AUTONOMOUS), SIVAKASI
DEPARTMENT OF CHEMISTRY

PG Programme – M.Sc. Chemistry

SEMESTER - III

ELECTIVE COURSE - II: DRUG DESIGN AND DISCOVERY (21PCH033)

(From 2021 – 2022 Batch onwards)

HOURS/WEEK: 6

CREDITS : 4

DURATION : 90 hrs

INT. MARKS : 40

EXT. MARKS : 60

MAX. MARKS : 100

Preamble

This course familiarize the students to learn the *in-silico* analysis of the drug through QASR, Docking methods and the importance of retrosynthetic analysis in the synthesis of drug

Course Outcomes (CO)

On successful completion of the course, the learners will be able to

CO1[K2]: express the various terms in pharmacology and its validation

CO2[K3]: apply the retrosynthetic method and computer aided designing in the drug synthesis

CO3[K4]: examine the various steps involved in drug discovery and its molecular interaction

CO4[K5]: deduce the structural activity of drug using QASR studies

CO5[K5]: evaluate the various physico-chemical parameters and predict the pharmacokinetics and pharmacodynamics mechanism and binding site of drugs

CO-PO Mapping table (Course Articulation Matrix)

PO CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1 [K2]	3	2	1	1	-	-	-
CO2 [K3]	3	2	1	1	1	1	1
CO3 [K4]	3	2	2	1	1	1	-
CO4 [K5]	3	3	2	1	1	-	1
CO5 [K5]	3	3	2	2	1	1	-
Weightage of the course	15	12	8	6	4	3	2
Weighted percentage of Course contribution to POs	5.05	5.02	5.19	5.5	5.19	3.85	3.17

Based on the level of contribution ('3'-High, '2'-Medium, '1'-Low '-' No Correlation)

UNIT I - DRUG DESIGN AND DISCOVERY

(18 hrs)

Historical Background –General terminologies – Drug Targets: Lipids, Carbohydrates, Proteins, Enzymes and Nucleic Acids as Drug Targets and Receptors - Receptor Pharmacology – Agonists and Antagonists (Partial and Full) - Allosteric Modulators. **Pharmacokinetics and Pharmacodynamics:** Administration, Absorption, Distribution, Metabolism, Elimination of Drugs-Bioavailability of Drugs - Side Effects.

UNIT II - DRUG IDENTIFICATION AND VALIDATION

(18 hrs)

Steps in Drug Discovery – Leads Identification- Hits- Drug Validation-Natural Products as Drugs – Molecular Recognition in Drug Design – Thermodynamic Considerations – Physical Basis and Inter Molecular Interactions Between Drugs and Targets Like Electrostatic Interactions – Ionic Bonds - hydrogen Bonds – Inductive Interactions – Dispersive Forces. Stereochemistry in Drug Designing - Stereospecificity of Drug Targets – Eudesmic Ratio – Examples of Eutomers and Distomers.

UNIT III - RETROSYNTHETIC STRATEGIES FOR DRUG SYNTHESIS (18 hrs)

Introduction to Retrosynthetic Analysis and Disconnection Approach – Synthons Acceptor and Donor – Synthetic Equivalents- Umpolungs – Planning a Synthesis – Relay and Convergent Routes - Guidelines For Disconnection – One Group C-X and C-C Disconnections – Chemoselectivity - Two Group C-C Disconnections in Dicarboxyls.

UNIT IV - COMPUTER AIDED DRUG DESIGN

(18 hrs)

Molecular Modeling in Drug Design – Energy Minimization Methods – Both Molecular Mechanics and Quantum Mechanical Methods –Energy Minimization – Conformational Analysis – Structure Based and Ligand Based Drug Design – QSAR – Parameters –Quantitative Models of QSAR – Hansch Methods – Free Wilson Model - 3D Pharmacophore Modeling – Docking – Rigid and Flexible Methods of Docking – Prediction of Binding Modes – Protein Ligand Binding Free Energies - Docking Score – Validation.

UNIT V - PHYSICO CHEMICAL PARAMETERS

(18 hrs)

: Solubility – Partition Coefficient – Ionization - pKa – Hydrogen bonding – Surface activity – Applications – Complexation – Redox potential – Steric features - Bioisosterism.

TEXTBOOKS:

1. Ratan kumar. *Fundamental of organic synthesis – The Retrosynthetic Analysis*. New Central Book Agencies (P) Ltd., Kolkata, 2008.

2. Ilango K., *Text book of Medicinal Chemistry Volume I*, Keerthi Publishers, Chennai, 2007.

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Books

1. Johann Gasteiger and Thomas Engel. *Cheminformatics*. Wiley-VCH, 2003.
2. Sg Wadodkar, Kasture A. V. *Pharmaceutical Chemistry-I*, Kindle Edition, 2015.

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1. <https://www.youtube.com/watch?v=Uc1dHNbCJWY>
2. <https://nptel.ac.in/courses/102/106/102106070/>
3. https://www.youtube.com/watch?v=yX_nPzmTpi8

SRI KALISWARI COLLEGE (AUTONOMOUS), SIVAKASI
DEPARTMENT OF CHEMISTRY
PG Programme – M.Sc. Chemistry
SEMESTER - III
SELF PACED LEARNING (SWAYAM COURSE): ADVANCED TRANSITION METAL
ORGANOMETALLIC CHEMISTRY (21PCHM31)
(From 2021 – 2022 Batch onwards)

CREDITS : 3

EXT. MARKS: 100

DURATION : 12 WEEKS

Preamble

This course provides the learners with an opportunity for a lifelong learning by meeting the demand in terms of knowledge, skills, and competencies.

Course Outcomes (CO)

On successful completion of the course, the learners will be able to

CO1[K1]: identify the background and the key words in Advanced Transition Metal Organometallic Chemistry

CO2[K2]: demonstrate independent and self-paced learning for clear understanding of the concept

CO3[K3]: develop computer and communication skills to broaden their knowledge in the course

CO4[K3]: use high quality reading resources, communication tools and technology to send assignments and to take up test

CO5[K4]: analyse critically and apply technical skills to comprehend the ideas or theories in the video lectures

CO-PO Mapping table (Course Articulation Matrix)

CO \ PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1[K1]	3	2	1	2	-	-	1
CO2[K2]	3	2	1	2	-	-	1
CO3[K3]	3	2	2	1	1	1	1
CO4[K3]	3	3	2	1	1	1	1
CO5[K4]	3	3	2	1	1	-	1
Weightage of the course	15	12	8	7	3	2	5
Weighted percentage of Course contribution to POs	5.05	5.02	5.19	6.42	3.9	2.56	7.94

Based on the level of contribution ('3'-High, '2'-Medium, '1'-Low '-' No Correlation)

COURSE LAYOUT

- Week 1:** s-, p-Donor/p-Acceptor Ligands, Allyl as Ligand, $C_3R_3^+$ as a Ligand
- Week 2:** Preparation and Properties of Transition Metal Complexes with C_4H_4 as a Ligand, C_5H_5 as a Ligand.
- Week 3:** Preparation and Properties of Transition Metal Cyclopentadiene Complexes, Cyclopentadienyl Metal Carbonyl Complexes.
- Week 4:** Transition Metal Cyclopentadienyl Carbonyl, Nitrosyl, Hydride and Halide Complexes
- Week 5:** C_6H_6 as a Ligand, Transition Metal Arene Complexes, Bis(arene)metal Complexes.
- Week 6:** Arene Transition Metal Carbonyl Complexes, Benzene Cyclopentadienyl Complexes, Complexes with C_7H_7 as a Ligand.
- Week 7:** Transition Metal Complexes with C_7H_7 and C_8H_8 as a Ligand, Metal p-Complexes of Heterocycles.
- Week 8:** C-C Cross Coupling Reactions, Heck Coupling, Suzuki Coupling, Stille Coupling.
- Week 9:** C-C Cross Coupling Reactions, Sonogashira Coupling Reactions, Hydrocyanation Reaction, C-Heteroatom Coupling, Hydroamination Reaction.
- Week10:** C-Heteroatom Coupling, hydroboration Reaction, Hydrosilylation Reaction, Olefin Oxidation Reactions.
- Week 11:** Water Gas Shift Reaction, Fischer-Tropsch Reaction, Carbonylation of Alcohols.
- Week12:** Hydrogenation of Alkene, Asymmetric Hydrogenation of Alkenes, Hydroformylation Reaction.

REFERENCE

Book

1. Elschenbroich (Organometallics), Crabtree (The Organometallic Chemistry of the Transition Metals).

SRI KALISWARI COLLEGE (AUTONOMOUS), SIVAKASI
DEPARTMENT OF CHEMISTRY
PG Programme – M.Sc. Chemistry
SEMESTER - III
SELF PACED LEARNING (SWAYAM COURSE): CHEMISTRY OF MAIN GROUP
ELEMENTS (21PCHM32)
(From 2021 – 2022 Batch onwards)

CREDITS : 3
DURATION: 12 WEEKS

EXT. MARKS: 100

Preamble

This course provides the learners with an opportunity for a lifelong learning by meeting the demand in terms of knowledge, skills, and competencies.

Course Outcomes (CO)

On successful completion of the course, the learners will be able to

- CO1[K1]:** identify the background and the key words in Chemistry of Main Group Elements
- CO2[K2]:** demonstrate independent and self-paced learning for clear understanding of the concept
- CO3[K3]:** develop computer and communication skills to broaden their knowledge in the course
- CO4[K3]:** use high quality reading resources, communication tools and technology to send assignments and to take up test
- CO5[K4]:** analyse critically and apply technical skills to comprehend the ideas or theories in the video lectures

CO-PO Mapping table (Course Articulation Matrix)

PO CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1[K1]	3	2	1	2	-	-	1
CO2[K2]	3	2	1	2	-	-	1
CO3[K3]	3	2	2	1	1	1	1
CO4[K3]	3	3	2	1	1	1	1
CO5[K4]	3	3	2	1	1	-	1
Weightage of the course	15	12	8	7	3	2	5
Weighted percentage of Course contribution to POs	5.05	5.02	5.19	6.42	3.9	2.56	7.94

Based on the level of contribution ('3'-High, '2'-Medium, '1'-Low '-' No Correlation)

COURSE LAYOUT

Week 1: Lecture 1: Classification of Elements and Periodic Properties

Lecture 2: Periodic Properties, Periodic Trends and Classification of main group Compounds

Lecture 3: Classification of Main Group Compounds

Lecture 4: Effective Nuclear Charge

Lecture 5: Structure and Bonding aspects: Lewis Structures and VSEPR Theory

Week 2: Lecture 6: Structure and Bonding Aspects: VSEPR Theory

Lecture 7: Structure and Bonding Aspects: Valence Bond Theory

Lecture 8: Structure and Bonding Aspects: Valence Bond Theory (contd...)

Lecture 9: Structure and Bonding Aspects: MO Theory

Lecture 10: Structure and Bonding Aspects: MO Theory (contd...)

Week 3: Lecture 11: Structure and Bonding Aspects: MO Theory (contd...)

Lecture 12: Structure and Bonding Aspects: MO Theory (contd...)

Lecture 13: Chemistry of Hydrogen

Lecture 14: Chemistry of Hydrogen (contd...)

Lecture 15: Chemistry of Hydrogen, Hydrides and Hydrogen Bonding

Week 4: Lecture 16: Chemistry of Group 1 Elements

Lecture 17: Chemistry of Group 1 Elements (contd...)

Lecture 18: Chemistry of Group 1 Elements (contd...)

Lecture 19: Chemistry of Group 1 Elements (contd...)

Lecture 20: Chemistry of Group 2 Elements

Week 5: Lecture 21: Chemistry of Group 2 Elements (contd...)

Lecture 22: Chemistry of Group 2 Elements (contd...)

Lecture 23: Chemistry of Group 2 Elements (contd...)

Lecture 24: Chemistry of Group 2 Elements (contd...)

Lecture 25: Chemistry of Group 13 Elements

Week 6: Lecture 26: Chemistry of Group 13 Elements (contd...)

Lecture 27: Chemistry of Group 13 Elements (contd...)

Lecture 28: Chemistry of Group 13 Elements (contd...)

Lecture 29: Chemistry of Group 13 Elements (contd...)

Lecture 30: Wades Rules

Week 7: Lecture 31: Chemistry of Group 13 Elements

Lecture 32: Chemistry of Group 14 Elements

Lecture 33: Chemistry of Group 14 Elements (contd...)

Lecture 34: Chemistry of Group 14 Elements (contd...)

Lecture 35: Chemistry of Group 14 Elements (contd...)

Week 8: Lecture 36: Chemistry of Group 14 Elements (contd...)

- Lecture 37: Chemistry of Group 14 Elements (contd...)
 Lecture 38: Chemistry of Group 14 Elements (contd...)
 Lecture 39: Chemistry of Group 15 Elements
 Lecture 40: Chemistry of Group 15 Elements (contd...)
- Week 9:** Lecture 41: Chemistry of Group 15 Elements (contd...)
 Lecture 42: Chemistry of Group 15 Elements (contd...)
 Lecture 43: Chemistry of Group 15 Elements (contd...)
 Lecture 44: Chemistry of Group 15 Elements (contd...)
 Lecture 45: Chemistry of Group 15 Elements (contd...)
- Week 10:** Lecture 46: Chemistry of Group 15 Elements (contd...)
 Lecture 47: Chemistry of Group 16 Elements
 Lecture 48: Chemistry of Group 16 Elements (contd...)
 Lecture 49: Chemistry of Group 16 Elements (contd...)
 Lecture 50: Chemistry of Group 16 Elements (contd...)
- Week 11:** Lecture 51: Chemistry of Group 16 Elements (contd...)
 Lecture 52: Chemistry of Group 17 Elements
 Lecture 53: Chemistry of Group 17 Elements (contd...)
 Lecture 54: Chemistry of Group 18 Elements
 Lecture 55: Chemistry of Group 12 Elements
- Week 12:** Lecture 56: Organometallic Compounds of Main Group Elements
 Lecture 57: Organometallic Compounds of Main Group Elements (contd...)
 Lecture 58: Organometallic Compounds of Main Group Elements (contd...)
 Lecture 59: Organometallic Compounds of Main Group Elements (contd...)
 Lecture 60: Overall Summary

REFERENCES

Books

1. F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann. *Advanced Inorganic Chemistry*. New York: John Wiley and Sons, 6th Edition, 1999.
2. D. F. Shriver and P. W. Atkins. *Inorganic Chemistry*, Oxford: Oxford University Press, 3rd Edition, 1999.
3. C. E. Housecroft and A. G. Sharpe. *Inorganic Chemistry*. Pearson, Prentice Hall 2nd Edition, 2005.
4. W. Henderson. *Main group chemistry*. Cambridge: Royal Society of Chemistry Publication, 2000.

SRI KALISWARI COLLEGE (AUTONOMOUS), SIVAKASI
DEPARTMENT OF CHEMISTRY
PG Programme – M.Sc. Chemistry
SEMESTER - IV
CORE COURSE - XIII: PHOTOCHEMISTRY, PERICYCLIC REACTIONS,
HETEROCYCLES AND NATURAL PRODUCTS (21PCHC41)
(From 2021 – 2022 Batch onwards)

HOURS/WEEK: 5
CREDITS : 5
DURATION : 75 hrs

INT. MARKS : 40
EXT. MARKS : 60
MAX. MARKS : 100

Preamble

This course familiarizes the learners with the photochemical and pericyclic reactions of organic compounds and the structural elucidation of natural products such as terpenoids and steroids.

Course Outcomes [CO]

On successful completion of the course, the learners will be able to

CO1[K2]: illustrate various organic photochemistry and pericyclic reaction

CO2[K3]: choose different methods to elucidate the structure of terpenoids, alkaloids and steroids

CO3[K4]: discriminate different types of photochemical and electrocyclic reactions and reactivity of heterocycles

CO4[K5]: critique the biological role of vitamins, Norrish type reaction, FMO approach the sigmatropic and cycloaddition reaction

CO5[K6]: elaborate the structure of terpenoids, steroids, vitamins and alkaloids.

CO-PO Mapping table (Course Articulation Matrix)

CO \ PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1 [K2]	3	2	1	1	1	-	-
CO2 [K3]	3	2	2	1	-	1	1
CO3 [K4]	3	3	2	1	1	1	1
CO4 [K5]	3	3	2	1	1	1	1
CO5 [K6]	3	3	3	1	1	-	1
Weightage of the course	15	13	10	5	4	3	4
Weighted percentage of course contribution to POs	5.05	5.44	6.49	4.59	5.19	3.85	6.35

Based on the level of contribution ('3'-High, '2'-Medium, '1'-Low '-' No Correlation)

UNIT I - ORGANIC PHOTOCHEMISTRY (15 hrs)

Principles of Photochemistry and Photochemical Reactions - Norrish type I & II Reactions - Paterno-Büchi Reaction - Photochemistry of Enones and Dienones - [2 + 2] Photochemical Cycloaddition - Photo Fries, di- π methane, oxa & aza, di- π Methane Rearrangements.

UNIT II - ORBITAL SYMMETRY AND PERICYCLIC REACTIONS (15 hrs)

Molecular Orbital and Orbital Symmetry of Diene System- FMO Approach- Electrocyclic Reaction - Stereochemistry - Cycloaddition Reaction- Diels-Alder Reaction and its Stereochemistry through FMO Approach. Sigmatropic Reactions- Cope Rearrangement - Claisen Rearrangement - Hydrogen Migration - Woodward and Hoffmann Rule for Pericyclic Reactions.

UNIT III - HETEROCYCLES AND THEIR REACTIVITY (15 hrs)

Structure, Synthesis and their Reaction of the Following Systems: One Heteroatom - Pyrrole - Furan - Thiophene - Pyridine - Benzo fused Heterocycles - Indole - Quinoline - Two Heteroatoms - Pyrazole - Imidazole - Pyrimidine - Pyrazine.

UNIT IV - NATURAL PRODUCTS: TERPENOIDS & STEROIDS (15 hrs)

Terpenoids: Isolation and Classification - General Methods to Elucidate the Structure of Terpenoids - Methods of Structure Elucidation and Synthesis - Zingiberine - Camphor - Eudesmol - Caryophyllene - Abietic Acid. Biosynthesis of Terpenes.

Steroids: Structural Elucidation - Cholesterol - Ergosterol- Vitamin-D - Equilenin - Estrone - Progesterone - Stigmasterol - Steroid Hormones - Androsterone - Testosterone. Biosynthesis of Steroids.

UNIT V - NATURAL PRODUCTS: ALKALOIDS AND VITAMINS (15 hrs)

Alkaloids: Structural Elucidation and Biosynthesis - Dictamnine - Chinconine - Morphine - Reserpine - Acronycine - Cocaine - Lysergic Acid - Nicotine.

Vitamins: Structure and Synthesis of Vitamins A₁, B₁, B₂, B₃, C, E and H - Biological Role of Vitamins.

TEXTBOOKS

1. Smith M. B. and Jerry March. *Advanced Organic Chemistry*. John Wiley & Sons, 5th Ed., 2001.

2. Sujata V. Bhat, B.A. Nagasampagi and S. Meenakshi. *Natural Products Chemistry and Applications*. Narosa Publishing House, 2009.
3. Jagdamaba Singh and Jaya Singh. *Photochemistry and Pericyclic reactions*. New Age International Publishers, 4th Edition, 2019.

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Books

1. Clayden J., Greeves N. and Warren S. *Organic Chemistry*. Oxford University Press, 2nd Ed., 2012.
2. Smith M. B. *Organic Synthesis*. Academic Press, 3rd Ed., 2011.
3. Gurdeep R. Chatwal. *Chemistry of Natural products Vol II*. Himalaya Publishing House, 2001.

Web Sources

1. <https://nptel.ac.in/courses/104/105/104105034/>
2. <https://www.slideshare.net/AhmedMetwaly3/alkaloids-lecture-1-introduction>
3. <https://nptel.ac.in/content/storage2/courses/104103022/download/module6.pdf>

SRI KALISWARI COLLEGE (AUTONOMOUS), SIVAKASI
DEPARTMENT OF CHEMISTRY

PG Programme – M.Sc. Chemistry

SEMESTER - IV

CORE COURSE - XIV: QUANTUM AND CHEMICAL KINETICS (21PCHC42)

(From 2021 – 2022 Batch onwards)

HOURS/WEEK: 5

CREDITS : 5

DURATION : 75 hrs

INT. MARKS : 40

EXT. MARKS : 60

MAX. MARKS : 100

Preamble

This course enables the students to gain knowledge in quantum mechanics and chemical kinetics.

Course Outcomes (CO)

On successful completion of the course, the learners will be able to

CO1[K2]: outline the fundamentals involved in the chemical kinetics and quantum mechanics

CO2[K2]: illustrate the basic concept of kinetics of fast and chain reactions, operators, approximation methods and salt effect of compounds

CO3[K3]: apply quantum mechanics to derive Schrodinger's wave equation for simple systems and approximation method to determine energy

CO4[K4]: examine the various types of quantum statistics and theories of kinetics

CO5[K5]: appraise the theories of quantum mechanics and chemical kinetics.

CO-PO Mapping table (Course Articulation Matrix)

PO CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1 [K2]	3	1	1	1	1	1	1
CO2 [K2]	3	2	1	1	1	1	-
CO3 [K3]	3	3	1	1	1	1	1
CO4 [K4]	3	3	2	1	1	1	1
CO5 [K5]	3	3	2	2	1	-	1
Weightage of the course	15	12	7	6	5	4	4
Weighted percentage of Course contribution to POs	5.05	5.02	4.55	5.5	6.49	5.13	6.35

Based on the level of contribution ('3'-High, '2'-Medium, '1'-Low '-' No Correlation)

UNIT I - APPLICATION OF QUANTUM MECHANICS

(15 hrs)

Derivation of Schrodinger Wave Equation – Application of SWE to Simple Systems – Free Particle Moving in One Dimensional Box – Particle Moving in 3D Box (Rectangular and Cubic Box) – Particle Moving in a Ring – Simple Harmonic Oscillator – Rigid Rotator – Spherical Harmonics – Hydrogen Atom Problem – Radial Wave Function – Radial Probability Distribution - Shapes of Various Atomic Orbitals.

UNIT II - APPROXIMATION METHODS IN QUANTUM MECHANICS

(15 hrs)

Need for Approximation Methods - Schrodinger Equation for He Atom and Other Many Electron System - Time Independent Perturbation Theory - First Order Correction Term for Energy and Wave Function (Derivation Required) - Application to Hydrogen Atom - Variation Theorem - Application to Hydrogen and He Atom- Hartree-Fock Self-Consistent Field (HFSCF) Method of Many Electron System and its Application to He Atom – Slater Determinants – Born-Oppenheimer Approximation – VB and MO Theories (Theory Only & Applications Not Included).

UNIT III - THEORIES OF KINETICS

(15 hrs)

: Effect of Temperature on Reaction Rate – Simple Collision Theory – Arrhenius Equation – Activated Energy and Chemical Reaction – Characteristics of an Activated Complex – Mathematical Treatment of Classical Collision Theory – Modified Collision Theory – ARRT – Statistical – Mechanical Derivation of the Rate Equation – Wyne – Joneand Erying Equation – Comparison of Collision Theory and Absolute Reaction Rate Theory.

UNIT IV - REACTION KINETICS

(15 hrs)

Unimolecular Reactions – Elementary Unimolecular Reactions – Unimolecular Reactions in Free Radical Mechanism – Theories of Unimolecular Reactions – Perrin Theory – Lindemann's Theory – Mathematical Formulation of Lindemann's Theory – Criticism of Lindemann's Theory – Hinshelwood's Theory – RRK Theory – RRKM Theory – Slater's Treatment – Trimolecular Reactions – Trauz's Theory – Bodenstein's Theory.

UNIT V - CHAIN REACTIONS

(15 hrs)

Distinguishing Features of Chain Reactions – Mechanism of Chain Reactions – Detection and Estimation of Atoms and Radicals in Chain Reactions – Kinetics of Chain Reactions – Steady State Treatment – Examples – Decomposition of Ozone – Reaction between Hydrogen and Bromine. **Salt Effect:** Primary and Secondary Salt Effect. **Kinetics of Fast Reactions:** Flow Methods – Flash Photolysis – Shock Tube – Pulse Radiolysis – Chemical Relaxation Method.

TEXTBOOKS

1. Puri B. R., Sharma L.R., Madan and S. Pathania. *Text Book of Physical Chemistry*. Jalandhar: Vishal Publishing and Co, 2008.
2. Prasad R. K. *Quantum Chemistry*. Jalandhar: New Age International Limited Publishers, 2015.
3. Levine N. *Quantum Chemistry*. Jalandhar: Printice Hall, 2003.
4. Laidler K. J. *Chemical Kinetics*. Jalandhar: Pearson Education, 2004.

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Books

1. Bajpai D. N. *Advanced Physical Chemistry*, New Delhi: S. Chand and Co. Private Limited, 2010.
2. Gurdeep Raj. *Advanced Physical Chemistry*. Jalandhar: GOEL Publication, 2012.
3. Donald A Mcquarrie. *Quantum Chemistry*. New Delhi: Viva Books Private Limited, 2005.

Web Sources

1. <https://www.youtube.com/watch?v=R-x9KdNjQmo>
2. <https://www.youtube.com/watch?v=c2SnT6a8juY>
3. <https://www.youtube.com/watch?v=7Ken5EC4OrU>
4. https://www.youtube.com/watch?v=zVEKh_mCGqw

SRI KALISWARI COLLEGE (AUTONOMOUS), SIVAKASI
DEPARTMENT OF CHEMISTRY
PG Programme – M.Sc. Chemistry
SEMESTER - IV
CORE COURSE - XV: RESEARCH METHODOLOGY (21PCHC43)
(From 2021 – 2022 Batch onwards)

HOURS/WEEK: 5
CREDITS : 4
DURATION : 75 hrs

INT. MARKS : 40
EXT. MARKS : 60
MAX. MARKS : 100

Preamble

This course enables the students to gain research knowledge in chemistry related to literature survey, chemistry softwares, and writing skills on thesis and research proposal.

Course Outcomes (CO)

On successful completion of the course, the learners will be able to

- CO1[K1]:** recognize the basic research ideas related to recent research, techniques and their methodologies
- CO2[K2]:** outline the basic concepts of research, literature survey and computer techniques in chemistry
- CO3[K3]:** apply the knowledge of fundamental concepts of chemistry in advanced research
- CO4[K4]:** simplify the outcome of instrumental method of analysis with the aid of chemistry softwares
- CO5[K5]:** appraise the ethics and art of science communication by developing the skill of effective thesis writing, paper writing and presentation in seminars and conferences.

CO-PO Mapping table (Course Articulation Matrix)

CO \ PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1 [K1]	3	2	1	1	1	1	1
CO2 [K2]	3	2	1	1	1	1	-
CO3 [K3]	3	2	2	1	1	1	1
CO4 [K4]	3	3	2	1	1	1	1
CO5 [K5]	3	3	2	2	1	1	1
Weightage of the course	15	12	8	6	5	5	4
Weighted percentage of Course contribution to POs	5.05	5.02	5.19	5.5	6.49	6.41	6.35

Based on the level of contribution ('3'-High, '2'-Medium, '1'-Low '-' No Correlation)

UNIT I - BASIC CONCEPTS OF RESEARCH (15 hrs)

Research-Definition and Types of Research (Descriptive vs Analytical; Applied vs Fundamental; Quantitative vs Qualitative; Conceptual vs Empirical). Research Methods vs Methodology. Literature Review and its Consolidation - Library Research - Field Research - Laboratory Research.

UNIT II - LITERATURE SURVEY (15 hrs)

Sources of Information - Primary Sources and Secondary Sources of Literature Survey - Journals Abbreviations - Importance of Journals - Impact Factor - h-Index - i-Index - ISSN - ISBN - Science Citation Index - Chemistry Journal Index. Computers in Literature Search Using Internet websites - American Chemical Society - Royal Society of Chemistry - Springer - Science Direct - Wiley - Interscience. Internet Search Engines - Google - Yahoo etc.,

UNIT III - COMPUTER TECHNIQUES IN CHEMISTRY (15 hrs)

Chemistry Software - Chemoffice - Chemdraw - Chem 3D & Chem Finder - Linear Regression - Multi Regression. MS Excel - Graph Drawing and Calculations. Origin - Rasmol - Visualization of Protein Molecules - Highlighting Amino Acids - Helices - Beta Sheets - Non-Hydrogen, Hydrogen and Sulphur Bonds - Identification of Metal Atoms and Active Sites. SHELX: Structure Solving and Refinement Using Shelxs and Shelxl. Key Chemistry Research Areas - Chemoinformatics.

UNIT IV - EFFECTIVE THESIS / RESEARCH REPORT WRITING (15 hrs)

Format of Research Report and Research Proposal - Style of Writing Report - Reports and Bibliography. Art of Writing a Thesis.

UNIT V - ETHICS AND ART OF SCIENTIFIC COMMUNICATION (15 hrs)

General Aspects of Scientific Writing - Reporting Practical and Project Work - Writing Literature Surveys and Reviews - Paper Writing for International Journals - Power Point Presentation - Poster Presentation - in Seminars & Conferences - Scientific Writing - Ethics - Plagiarism.

TEXTBOOKS

1. Barbara Kasser. *Using the Internet*. New Delhi: 4th Ed., 1998.
2. Abdul Rahim F. *Thesis Writing, A Manual Researcher*. New Delhi: New Age International Ltd, 1996.
3. Peter C Jurs. *Computer Software Applications in Chemistry*. Wiley Interscience, 2nd Edition, 1996.

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1. Dawson C. *Practical Research Methods*. New Delhi: UBS Publishers, 2002.
2. Geffery G. H, Basselt J., Mendhan and Denney R. C. *Vogel's Text Book of Quantitative Chemical Analysis*. UK: Longman Scientific and Industrial, 5th Edition, 1989.
3. Anderson J., Durston B. H. and Poole M. *Thesis and Assignment Writing*. New Delhi: Wiley Eastern Ltd, 1997.

Web Sources

1. <https://nptel.ac.in/courses/121/106/121106007/>
2. <https://www.youtube.com/watch?v=Yzfl3rtF0SM>
3. <https://www.youtube.com/watch?v=vHHtfO-Bu1M>
4. <https://nptel.ac.in/courses/102/104/102104061/>
5. <https://nptel.ac.in/noc/courses/noc20/SEM1/noc20-bt05/>

SRI KALISWARI COLLEGE (AUTONOMOUS), SIVAKASI
DEPARTMENT OF CHEMISTRY

PG Programme – M.Sc. Chemistry

SEMESTER - IV

CORE COURSE - XVI: PROJECT (21PCHJ41)

(From 2021 – 2022 Batch onwards)

HOURS/WEEK: 15

CREDITS : 4

DURATION : 225 hrs

INT. MARKS : 50

EXT. MARKS : 50

MAX. MARKS : 100

Preamble

This course gives exposure to learners to perform literature survey, apply chemistry software, synthesis of compounds in lab and analyse the sample through the instrumentation techniques.

Course Outcomes (CO)

On successful completion of the course, the learners will be able to

CO1[K2]: demonstrate research ideas related to recent research through literature survey

CO2[K3]: perform research work based on the knowledge acquired from research papers

CO3[K4]: discriminate the products formed in synthetic work on the basis of characterisation by instrumentation techniques

CO4[K5]: judge the result of research work and propose the mechanism of the reaction

CO5[K6]: develop scheme for research in future, skill in thesis writing and publication of research work in reputed journals.

CO-PO Mapping table (Course Articulation Matrix)

CO \ PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1 [K2]	3	2	1	1	1	1	1
CO2 [K3]	3	2	1	1	1	1	1
CO3 [K4]	3	2	2	1	1	1	1
CO4 [K5]	3	3	2	1	1	1	1
CO5 [K6]	3	3	2	1	2	-	1
Weightage of the course	15	12	8	5	6	4	5
Weighted percentage of Course contribution to POs	5.05	5.02	5.19	4.59	7.79	5.13	7.94

Based on the level of contribution ('3'-High, '2'-Medium, '1'-Low '-' No Correlation)

Project Work Guidelines

1. Students are required to submit a project at the end of the IV semester. The student will work under a faculty member as the research guide.
2. Depending on the interest of the students, project research areas will be chosen.
3. Students must meet the guide periodically.
4. The project carries 100 marks of which 50 marks for Internal Assessment and 50 Marks for External Examination.
5. There will be two project review sessions.
6. Each student must either present paper or participate in Conferences/Seminars related to his Project work.
7. A draft of the final project report should be submitted to the Project Guide for review atleast three weeks prior to the end of the semester.
8. The project report should be of minimum 40/50 pages (excluding bibliography & appendices)
9. Three copies of the final project report should be submitted.
10. The Head of the department and the Project Guide will evaluate the final Project Report.
11. The viva voce board shall consist of the External Examiner, the Head of the Department and the Internal Examiner (Research Project Guide)

The following rubrics will be taken into account for the evaluation of Project work and viva-voce:

Internal Assessment (50 Marks)

Project Report & Review	: 40 Marks
PowerPoint Presentation	: 5 Marks
Participation/Publications in Conferences or Seminars	: 5 Marks

External Examination (50 Marks)

Project Report	: 20 Marks
Viva Voce	: 30 Marks