SACRED HEART COLLEGE (AUTONOMOUS)

THEVARA, KOCHI – 682013

KERALA

CURRICULUM AND SYLLABUS

of

M.Sc. CHEMISTRY

(PG CREDIT SEMESTER SYSTEM)

CHOICE BASED CREDIT AND SEMESTER SYSTEM (CBCSS)

INTRODUCED FROM 2024 ADMISSION ONWARDS

Prepared by:

Board of Studies in Chemistry

Sacred Heart College (Autonomous)

Thevara

BOARD OF STUDIES IN CHEMISTRY

Sacred Heart College (Autonomous) Thevara, Kochi, Kerala

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17	**Dr. Jaison M Joy** Assistant Professor Sacred Heart College, Thevara.	Faculty member
18	**Dr. Shalumon K T** Assistant Professor Sacred Heart College, Thevara.	Faculty member
19	**Dr. Thomasukutty Jose** Assistant Professor Sacred Heart College, Thevara.	Faculty member

PREFACE

I am greatly privileged in presenting the revised curricula and syllabi of M.Sc. Chemistry for the approval of Faculty, Board of Studies and Academic Council of Sacred Heart College (Autonomous) Thevara.

Chemistry is a fundamental science and has contributed immensely for the improvement of human life by providing materials, methods and other essentialities. Also, chemistry is essential to solve many future problems, including sustainable energy and food production, managing our environment, providing safe drinking water and promoting human and environmental health. The progress achieved in the fields of chemistry in the past few decades was phenomenal. It is also seen that these developments are crossing the traditional vertical boundaries of scientific disciplines. Now a chemist cannot isolate himself from other disciplines. New branches of chemistry such as computational chemistry, bioorganic chemistry, material chemistry, green chemistry etc. are emerging and gaining importance. The practise of chemistry in industry is also undergoing radical changes. It is with these visions we have revised the syllabi of the two PG courses. Also, we have followed the PG Guidelines prepared by Mahatma Gandhi University, Kottayam in this attempt. The revised syllabi will be implemented with effect from academic year 2024-25 and onwards under Choice Based Credit System (CBCS).

The PG Board of Studies in Chemistry was entrusted with the duty of preparing the revised curricula and syllabi for the two M.Sc. Programmes in Chemistry currently approved by the Mahatma Gandhi University. The BoS has taken keen interest in collecting expert opinion from the renowned experts in the field as well as from the faculties of the affiliated colleges handling the subjects. We have also referred to the syllabi of various Central Universities, IISERs, IITs and the UGC model curriculum in this attempt.

The revised syllabus is prepared based on Outcome Based Education (OBE). Programme Specific Objectives (PSO) for the MSc Chemistry programme and Course Outcomes (CO) for each course have been prepared for effective teaching-learning process.

The BoS prepared draft proposals of revised curricula and syllabi for the two M.Sc. Programmes in Chemistry keeping the Credit and Semester System. The syllabus has been set with an objective of training the students in all the fundamentals of the subject along with good practical exposure. Most of the advanced topics have been incorporated in the fourth semester. In view of creating research aptitude in students, BoS has decided to give sufficient time (three months) for project work. Thus, students could get admission in reputed research centres/Universities in and outside the state for doing their project.

The BoS feels that appreciable updating could be done considering the current developments and latest trends in chemistry education. The task of preparing the Curricula and Syllabi and bringing it out in the present form was not a simple task but it was possible with the dedicated efforts, wholehearted support and involvement of all the members of the faculty and BoS. I would like to express my sincere thanks to all my fellow members of the BoS and faculty for all their help, cooperation and encouragement.

Dr. Franklin J
Chairman
PG & UG Board of Studies
Sacred Heart College (Autonomous), Thevara.

CONTENTS

1. INTRODUCTION

1.1 M.Sc. Chemistry Programme

Chemistry-the 'central science' is about the nature of matter, how to make it, how to measure it and how to model it. In that sense chemistry really matters; it is essential to explaining all the real world. The M.Sc. Chemistry programme is a two year – four semester programme. The programme intends to expand and deepen student's knowledge in the main topic areas such as inorganic chemistry, organic chemistry, physical chemistry, analytical chemistry and theoretical chemistry. Student will gain deeper understanding of the subject and flair of research through lectures, laboratory sessions, assignments, seminars and project works. This programme combines theory, practical and project work to develop skills in demand by industry, or prepare for further research study.

1.2 Eligibility for Admissions:

Graduation in Chemistry/ Petrochemicals with not less than 50% marks or equivalent grade in Part III subjects (Main/Core + subsidiaries/Complementaries).

2.1 TITLE

These regulations shall be called '**SACRED HEART COLLEGE REGULATIONS FOR POST GRADUATE PROGRAMMES UNDER CREDIT SEMESTER SYSTEM (CSS) – 2024'**

2.2 SCOPE

Applicable to all Post Graduate (PG) programmes of the college with effect from 2024 admissions. The provisions herein supersede all the existing regulations for the Post Graduate programmes of the college.

2.3 DEFINITIONS

2.3.1 '**Programme**' means the entire course of study and examinations.

2.3.2 **Duration of Programme'** means the period of time required for the conduct of the programme. The duration of post-graduate programme shall be of 4 semesters and M Phil programmes shall be 2 semesters.

2.3.3 **'Semester'** means a term consisting of a minimum of 90 working days, inclusive of examination, distributed over a minimum of 18 weeks of 5 working days, each with 5 contact hours of one hour duration

2.3.4 **'Course'** means a segment of subject matter to be covered in a semester. Each Course is to be designed variously under lectures / tutorials / laboratory or fieldwork/ study tour /seminar / project / practical training / assignments/evaluation etc., to meet effective teaching and learning needs.

2.3.5 **'Credit' (Cr)** of a course is the numerical value assigned to a course according to the relative importance of the content of the syllabus of the programme.

2.3.6 '**Extra credits**' are additional credits awarded to a student over and above the minimum credits required for a programme.

2.3.7 '**Programme Credit'** means the total credits of the PG Programmes. For PG programmes the total credits shall be 80.

2.3.8 **'Programme Elective Course'** means a course, which can be chosen from a list of electives and a minimum number of courses is required to complete the programme.

2.3.9 **'Elective Group'** means a group consisting of elective courses for the programme.

2.3.10 '**Programme Project'** means a regular project work with stated credits on which the student undergoes a project under the supervision of a teacher in the parent department / any appropriate Institute in order to submit a dissertation on the project work as specified.

2.3.11 '**Internship**' is on-the-job training for professional careers.

2.3.12 '**Plagiarism**' Plagiarism is the unreferenced use of other authors' material in dissertations and is a serious academic offence.

2.3.13 '**Seminar'** seminar means a lecture by a student expected to train the student in self-study, collection of relevant matter from the books and Internet resources, editing, document writing, typing and presentation.

2.3.14 '**Evaluation'** means every course shall be evaluated by 25% continuous (internal) assessment and 75% end course/end semester (external) assessment.

2.3.15 '**Repeat Course'** is a course that is repeated by a student for having failed in that course in an earlier registration.

2.3.16 **'Audit Course'** is a course for which no credits are awarded.

2.3.17 '**Department'** means any teaching Department offering a course of study approved by the college / Institute as per the Act or Statute of the University.

2.3.18 '**Department Council'** means the body of all teachers of a Department in a College.

2.3.19 **'Faculty Advisor'** is a teacher nominated by a Department Council to coordinate the continuous evaluation and other academic activities undertaken in the Department.

2.3.20 '**College Co-ordinator'** means a teacher from the college nominated by the College Council to look into the matters relating to CSS-PG System.

2.3.21 **'Letter Grade'** or simply '**Grade**' in a course is a letter symbol (A^+, A, B^+, B etc.) which indicates the broad level of performance of a student in a course.

2.3.22 **'Grade point'** (GP) which is an integer indicating the numerical equivalent of the broad level of performance of a student in a course.

2.3.23 **'Weighted Grade Point**' (WGP) is obtained by multiplying the grade point by its weight (WGP = GP × weight).

2.3.24 **'Grade Point Average' (GPA)** is an index of the performance of a student in a course. It is obtained by dividing the sum of the weighted grade points obtained in the course by the sum of the weights of the course (GPA = ∑WGP/∑W).

2.3.25 **'Credit Point'** (CP) of a course is the value obtained by multiplying the grade point (GP) by the Credit (Cr) of the course (CP = GPA × Cr).

2.3.26 '**Semester Grade Point Average'** (SGPA) is the value obtained by dividing the sum of credit points (CP) obtained by a student in the various courses taken in a semester by the total number of credits taken by him/her in that semester . The grade points shall be rounded off to two decimal places. SGPA determines the overall performance of a student at the end of a semester.

2.3.27 **'Cumulative Grade Point Average'** (CGPA) is the value obtained by dividing the sum of credit points in all the courses taken by the student for the entire programme by the total number of credits and shall be rounded off to two decimal places.

2.3.28 **'Grace Grade Points'** means grade points awarded to a student for course(s), in recognition of meritorious achievements in NSS/Sports/Arts and cultural activities, as per the orders issued by the college from time to time.

2.4 <u>ATTENDANCE</u>

Being a regular college, physical presence in the regular activities, especially, classes and exams, is mandatory for the students. However, if a student secures 75% of attendance he/she is eligible to appear for the exams, provided there are no other impediments like disciplinary proceedings, malpractice record etc.

2.4.1 **Absence:** A student found absent for one hour in the forenoon or afternoon session is deprived of the attendance for the entire session as far as eligibility for final exam is concerned.

2.4.2 **Leave**: A student has to formally report his/her absence with reasons either in advance, or immediately after the absence for obtaining an approved leave. This applies to all sorts of leave – medical, on duty or similar cases.

2.4.3 The student has to retain a copy/section of the approved leave form and produce the same as proof, in case there is any confusion regarding the leave sanctioning. In the absence of such proof, the claims will not be entertained.

2.4.4 **Duty Leave**: A student representing the college in sports, arts, social service or academic matters, has to get sanction from the class teacher concerned and submit the leave application form duly endorsed by the class teacher and the Head of the Department, and submit it to the Vice Principal. The same will be forwarded by the Vice Principal for attendance entry.

The approval of the Department of Physical Education and the class teacher is required for granting attendance related to sports. The time limit for submission mentioned above is applicable in the case of duty leave as well.

2.4.5 **Condonation**: A student may have the privilege of condonation of attendance shortage (up to a maximum of ten days) on the basis of genuineness of the grounds of absence (medical reasons or college duty), duly recommended by the department. This is not a matter of right. It is a matter of privilege based on Principal's discretion and the good conduct of the student on the campus. A student of PG programme may have only one such opportunity.

2.4.6 **Re-admission**: A student whose attendance is inadequate will have to discontinue the studies. Such students, whose conduct is good, may be re-admitted with the approval of Governing Body, on the basis of recommendation from the department, and assurance from the student and the guardian regarding good conduct and compliance in academic and discipline matters. For this the prescribed re-admission fee has to be paid.

2.4.7 **Unauthorized absence & removal from rolls**: A student, absent from the classes continuously for ten consecutive working days without due intimation or permission, shall be removed from the rolls, and the matter shall be intimated to the student concerned. On the basis of recommendation of the department concerned, re-admission process may be permitted by the Principal.

2.5 PROGRAMME REGISTRATION

2.5.1 A student shall be permitted to register for the programme at the time of admission.

2.5.2 A PG student who registered for the programme shall complete the same within a period of 8 continuous semesters from the date of commencement of the programme.

2.6 PROMOTION

A student who registers for the end semester examination shall be promoted to the next semester. However, in extreme circumstances, a student having sufficient attendance who could not register for the end semester examination may be allowed to register notionally by the Principal with the recommendation of the Head of the Department concerned and by paying the prescribed fee.

2.7 EXAMINATIONS

All the End Semester Examinations of the college will be conducted by the Controller of Examination. The Principal will be the Chief Controller of Examinations. An Examination committee consisting of the Chief Controller of Examinations, Controller of Examinations, Additional Chief Superintendent, Deans, IQAC Coordinator and other faculty members nominated by the Principal will act as an advisory body on the matters relating to the conduct of examinations.

2.8 EVALUATION AND GRADING

2.8.1 Evaluation:

The evaluation scheme for each course shall contain two parts;

(a) Continuous Internal Assessment (CIA) and

(b) End Semester Examination (ESE).

25% weightage shall be given to internal evaluation and the remaining 75% to external evaluation and the ratio and weightage between internal and external is **1:3**, for the courses with or without practicals (except the courses offered by the School of Communications). In the case of courses offered by the School of Communications, the internal-external assessment ratio shall be **1:1**. In their case, the components for evaluation and their respective weightage shall be determined by their Board of Studies. Both internal and external evaluation shall be carried out in the grading system and the GPAs are to be rounded to two places of decimals.

2.8.2 Direct Grading:

The direct grading for the components of CIA shall be based on six letter grades (A+, A, B, C, D and E) with numerical values of 5, 4, 3, 2, 1 and 0 respectively as per the following scale of accuracy/level of quality. The questions for internal test papers and the end semester examination shall be prepared in such a way that the answers can be awarded A+, A, B, C, D and E grades.

Grade	Grade Points	Scale of Accuracy/Level of quality
A+	5	Greater than or equal to 90%
A	4	80% to less than 90%
B	3	60% to less than 80%
C	2	40% to less than 60%
D	1	20% to less than 40%
E	0	Less than 20%

2.8.3 Grade Point Average (GPA): Internal and external components are separately graded and the combined GPA shall be calculated for each course with weightage **1** for internal and **3** for external.

2.8.4 Continuous Internal Assessment (CIA)/ Continuous Assessment:

Grades shall be given to the evaluation of theory/practical/project/comprehensive viva-voce and all internal evaluations are based on the Direct Grading System.

a) Components of Internal Evaluation (for theory)

Sl. No.	Components	Weightage
i.	Assignments	1
ii.	Seminar	1
iii.	Quiz/Field study/Industrial Visit/Viva Voce/Study Tour	1
iv.	Test paper-1	1
v.	Test paper-2	1
	Total	**5**

b) Components of Internal Evaluation (for Practical)

Sl. No.	Components	Weightage
i.	Written / Lab Test	2
ii.	Record	1
iii.	Lab Involvement	1
iv.	Viva	1
	Total	**5**

c) Components of Internal Evaluation (for Project)

Sl. No.	Components	Weightage
i.	Relevance of the topic and analysis	2
ii.	Project content and presentation	2
iii.	Project viva-voce	1
	Total	**5**

d) Components of Internal Evaluation (for Comprehensive Viva-Voce)

Sl. No.	Components	Weightage
i.	Comprehensive viva voce (all courses from first semester to fourth semester)	5
	Total	**5**

2.8.5 Components of End Semester Examination (ESE):

a) For Theory

Evaluation shall be based on the following pattern of questions:

Sl. No.	Type of Question	Weight	Number of Questions to be answered
i.	Short answer type	1	8 out of 10
ii.	Short Essay / Problem Solving type	2	6 out of 8
iii.	Long Essay / Problem solving type	5	2 out of 4

b) Components of External Evaluation (for Practical)

Sl. No.	Components	Weightage
i.	Written / Lab Test	10
ii.	Record	2
iii.	Viva	3
	Total	**15**

c) Components of External Evaluation (for Project)

Sl. No.	Components	Weightage
i.	Relevance of the topic and analysis	3
ii.	Project content and presentation	7
iii.	Project viva-voce	5
	Total	**15**

d) Components of External Evaluation (for Comprehensive Viva-Voce)

Sl. No.	Components	Weightage
i.	Comprehensive viva voce (all courses from first semester to fourth semester)	15
	Total	**15**

2.8.6 Project: Project work is a part of the syllabus of most of the programmes offered by the college. The guidelines for doing projects are as follows:

i. Project work shall be completed by working outside the regular teaching hours.

ii. Project work shall be carried out under the supervision of a teacher in the concerned department or an external supervisor.
iii. A candidate may, however, in certain cases be permitted to work on the project in an industrial / Research Organization/ Institute on the recommendation of the Supervisor.
iv. There should be an internal assessment and external assessment for the project work in the ratio 1:3
v. The external evaluation of the project work consists of valuation of the dissertation (project report) followed by presentation of the work and viva voce.

2.9 PERFORMANCE GRADING

2.9.1 Students are graded based on their performance (GPA/SGPA/CGPA) at the examination on a 7 point scale as detailed below

Range	Grade	Indicator
4.50 to 5.00	**A+**	**Outstanding**
4.00 to 4.49	**A**	**Excellent**
3.50 to 3.99	**B+**	**Very Good**
3.00 to 3.49	**B**	**Good (Average)**
2.50 to 2.99	**C+**	**Fair**
2.00 to 2.49	**C**	**Marginal (Pass)**
Up to 1.99	**D**	**Deficient (Fail)**

2.9.2 ***No separate minimum i***s required for internal evaluation for a pass, but a minimum a 'C' grade is required for a pass in an external examination. However, a minimum 'C' grade is required for pass in a course and the programme as well.

2.9.3 A student who fails to secure a minimum grade 'C' for a pass in a course shall be permitted to write the examination along with the next batch.

2.9.4 ***Improvement of GPA***: The candidates who wish to improve the GPA of the external examinations of a course/courses can do the same by appearing in the external examination of the semester concerned along with the immediate junior batch. The facility is restricted to first and second semesters of the programme.

2.9.5 ***Computation of SGPA and CGPA***: For the successful completion of a semester, a student should pass all the courses and score at least the minimum SGPA grade 'C'. After the successful completion of a semester, Semester Grade Point Average (SGPA) of a student in that semester is calculated as the ratio of the sum of the credit points of all courses taken by a student in the semester to the total credits of that semester.

Thus, $SGPA = {TCP}/{TCr}$ $\boldsymbol{i=1}$

Where, **TCP** is Total Credit Point of that semester $\left(\sum_{i=1}^{n} CP_i\right)$;

TCr is Total Credit of that semester $\left(\sum_{i=1}^{n} Cr_i\right)$ and

'*n*' is the number of courses in that semester.

Computation of CGPA: Cumulative Grade Point Average (CGPA) of a programme is calculated as the ratio of the sum of the credit points of all the courses of the programme to the total credits of the programme.

$$CGPA = \frac{\sum(SGPA \times TCr)}{\sum TCr}$$

The SGPA/CGPA shall be rounded off to two decimal places.

For the successful completion of a programme, a student should pass all the courses and score at least the minimum CGPA grade 'C'. However, a student is permitted to move to the next semester irrespective of her/his SGPA.

To ensure transparency of the evaluation process, the internal assessment grade awarded to the students in each course in a semester shall be published on the notice board/website at least one week before the commencement of external examination. There shall not be any chance for improvement for internal assessment grade.

The course teacher and the faculty advisor shall maintain the academic record of each student registered for the course which shall be forwarded to the controller of examinations through the Head of the Department and a copy should be kept in the department for at least two years for verification.

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2.10 <u>REGISTRATION FOR THE EXAMINATION</u>

a. All students admitted in a programme with remittance of prescribed fee are eligible for the forthcoming semester examinations.
b. Online application for registration to the various End Semester Examinations shall be forwarded to the CE along with prescribed fee for each course in prescribed format.
c. The eligible candidates who secure the prescribed minimum attendance of the total duration

of the course and possess other minimum qualification prescribed in the regulations for each course shall be issued the hall tickets. The hall ticket shall be downloaded by the students from the college website.

d. The mode of fee remittance shall be through the prescribed bank.

2.11 SUPPLEMENTARY EXAMINATIONS

Candidates who failed in an examination can write the supplementary examination conducted by the College along with regular examinations.

2.12 PROMOTION TO THE NEXT HIGHER SEMESTER

A candidate shall be eligible for promotion from one semester to the next higher semester if,

a) He / she secures a minimum 75 % attendance and registered for the End Semester Examination of the programme for which he/she is studying.

b) His / her progress of study and conduct are satisfactory during the semester completed, as per the assessments recorded by the course teachers and the Head of the Department concerned.

2.13 CERTIFICATES

1. Diploma and Degree certificates are issued by the Mahatma Gandhi University, Kottayam as per the act and statues of the University on the submission of the consolidated mark / score cards of the students by the College.
2. A consolidated mark / scored card shall be issued to the candidates after the publication of the results of the final semester examination taken by the candidate.
3. A Course Completion Certificate with classification shall be issued to students till the provisional certificate is issued by the university.

2.14 RANK CERTIFICATE

Candidates shall be ranked in the order of merit based on the CGPA secured by them. Grace grade points awarded to the students shall not be counted for fixing the rank/positions. Rank certificates shall be issued to the candidates who secure positions from the first to the third in the order of merit. The position certificates shall be issued to the next seven candidates in the order of merit.

2.15 AWARD OF DEGREE

The successful completion of all the courses with **'C'** grade shall be the minimum requirement for the award of the degree.

2.16 MONITORING

There shall be a Monitoring Committee constituted by the Principal consisting of faculty advisors, HoD, a member from Teaching Learning Evaluation Committee (TLE) and the Deans to monitor the internal evaluations conducted by college. The course teacher, class teacher and the deans should keep all the records of the internal evaluation, for at least a period of two years, for verification.

Every programme conducted under Credit Semester System shall be monitored by the College Council under the guidance of IQAC Coordinator, Controller of Exams, Academic Deans and HoDs. An academic committee consisting of the vice principal, deans and teachers nominated by the Principal shall look after the day-to-day affairs of these regulations.

2.17 GRIEVANCE REDRESSAL MECHANISM

In order to address the grievance of students regarding Continuous Internal Assessment (CIA) a three-level grievance redressal mechanism is envisaged. A student can approach the upper level only if grievance is not addressed at the lower level.

Level 1: Level of the course teacher concerned

Level 2: Level of a department committee consisting of the Head of the Department, a coordinator of internal assessment for each programme nominated by the HoD and the course teacher concerned.

Level 3: A committee with the Principal as Chairman, Dean of the Faculty concerned, HOD of the department concerned and one member of the Academic Council nominated by the Principal every year as members

2.18 TRANSITORY PROVISION

Notwithstanding anything contained in these regulations, the Principal of the college has the power to make changes in these regulations, by due orders, that shall be applied to any programme with such modifications as may be necessary on the recommendations of the Board of Studies of the respective programme.

PROGRAMME STRUCTURE

Course Code	Course Title	Credits	Hours / Week	Hour / Sem.
	SEMESTER I			
24P1CHET01	Inorganic Chemistry - I	4	4	72
24P1CHET02	Basic Organic Chemistry	4	4	72
24P1CHET03	Physical Chemistry – I	3	3	54
24P1CHET04	Quantum Chemistry & Group Theory	4	4	72
24P2CHEP01	Inorganic Chemistry Practical - I	-	3	54
24P2CHEP02	Organic Chemistry Practical - I	-	3	54
24P2CHEP03	Physical Chemistry Practical - I	-	4	72
	Total	**15**	**25**	**450**
	SEMESTER II			
24P2CHET05	Inorganic Chemistry - II	4	4	72
24P2CHET06	Organic Reaction Mechanism	4	4	72
24P2CHET07	Physical Chemistry - II	3	3	54
24P2CHET08	Theoretical & Computational Chemistry	4	4	72
24P2CHEP01	Inorganic Chemistry Practical - I	3	3	54
24P2CHEP02	Organic Chemistry Practical - I	3	3	54
24P2CHEP03	Physical Chemistry Practical - I	3	4	72
	Total	**24**	**25**	**450**
	SEMESTER III			
24P3CHET09	Inorganic Chemistry - III	4	4	72
24P3CHET10	Organic Syntheses	4	4	72
24P3CHET11	Physical Chemistry - III	4	4	72
24P3CHET12	Spectroscopic Methods in Chemistry	3	3	54
24P4CHEP04	Inorganic Chemistry Practical – II	-	3	54
24P4CHEP05	Organic Chemistry Practical – II	-	3	54
24P4CHEP06	Physical Chemistry Practical - II	-	4	72
	Total	**15**	**25**	**450**
	SEMESTER IV			
24P4CHET13EL	Advanced Inorganic Chemistry	4	5	90
24P4CHET14EL	Advanced Organic Chemistry	4	5	90
24P4CHET15EL	Advanced Physical Chemistry	4	5	90
24P4CHEP04	Inorganic Chemistry Practical – II	3	3	54
24P4CHEP05	Organic Chemistry Practical – II	3	3	54
24P4CHEP06	Physical Chemistry Practical – II	3	4	72
24P4CHECV	Comprehensive Subject Viva Voce	2	-	-
24P4CHEPJ	Project Viva	3	-	-
	Total	**26**	**25**	**450**

Programme outcomes for the Postgraduate Students of Sacred Heart College, Kochi

At the end of the PG programme,

PO 1	The students are capable of exercising their critical thinking in creating new knowledge leading to innovation, entrepreneurship and employability.
PO 2	The students are able to effectively communicate the knowledge of their study and research in their respective disciplines to their employers and to the society at large.
PO 3	The students are able to make choices based on the values upheld by the college, and have the readiness and know-how to preserve environment and work towards sustainable growth and development.
PO 4	The students possess an ethical view of life, and have a broader (global) perspective transcending the provincial outlook.
PO 5	The students possess a passion for exploring new knowledge independently for the development of the nation and the world and are able to engage in a lifelong learning process.

Programme Specific Outcomes of MSc Chemistry

At the end of M.Sc. Chemistry Programme, the student should be able to:

Knowledge and Understanding	
PSO1	Demonstrate an in-depth knowledge and understanding of the principles of Inorganic, Organic, Physical and Theoretical Chemistry.
PSO2	Demonstrate an awareness of the relevance of chemistry in a wider multi-disciplinary context.
Intellectual Abilities	
PSO3	Apply their understanding in Chemistry to design solutions to unfamiliar problems in Chemistry and those involving other related disciplines.
PSO4	Use their knowledge and understanding to conceptualize appropriate models and representations.
Practical Skills	
PSO5	Design and conduct analytical, modelling and experimental investigations in Inorganic, Organic, Physical and Theoretical Chemistry.
Professional Skills	
PSO6	Ability to identify, design and conduct appropriate experiments, interpret data obtained, draw pertinent conclusions and communicate all these effectively.

III

SYLLABUS OF THE COURSES

SEMESTER I

24P1CHET01: INORGANIC CHEMISTRY-I

Credits: 4 **Contact Lecture Hours: 72**

After completing the course, the students will be able to:

	Course Outcome	*POs / PSOs*	*CL*	*KC*	*Class Sessions*
CO1	Describe the key concepts of inorganic and organometallic chemistry including those related to synthesis, reaction chemistry, and structure and bonding.	PO 1 PSO 1	U	F	27
CO2	Explain stability of organometallic compounds and clusters, and their application as industrial catalysts.	PO 1 PSO 4	A	C	18
CO3	Recognize and explain the interaction of different metal ions with biological ligands.	PO 1 PSO 1	U	F	18
CO4	Demonstrate a systematic understanding of the key aspects of nuclear chemistry and their analytical applications.	PO 1 PSO 1	U	F	9

Unit 1: Organometallic Compounds - Synthesis, Structure and Bonding **(18 Hrs)**

1.1 Hapto nomenclature of organometallic compounds, organometallic compounds with linear *pi*-donor ligands-olefins, acetylenes, dienes and allyl complexes-synthesis, structure and bonding.

1.2 Synthesis and structure of complexes with cyclic *pi*-donors, metallocenes and cyclic arene complexes, bonding in ferrocene and dibenzenechromium, carbene and carbyne complexes.

1.3 *Metal carbonyls*: CO as a π-bonding ligand, synergism, preparation, properties, structure and bonding of simple mono and binuclear metal carbonyls, metal nitrosyls, metal cyanides and dinitrogen complexes. Polynuclear metal carbonyls with and without bridging. Carbonyl clusters - LNCCS and HNCCS, Isoelectronic and isolobal analogy, Wade-Mingos rules, cluster valence electrons. IR spectral studies of bridging and non-bridging CO ligands.

Unit 2: Reactions of Organometallic Compounds **(9 Hrs)**

2.1 Substitutio*n* reactions - nucleophilic ligand substitution, nucleophilic and electrophilic attack on coordinated ligands.

2.2 Addition and elimination reactions - 1,2 additions to double bonds, carbonylation and decarbonylation, Oxidative addition - concerted addition, S_N2, radical and ionic mechanisms. Reductive elimination- binuclear reductive elimination. Oxidative coupling and reductive decoupling. Insertion (migration) and elimination reactions – insertions of CO and alkenes, insertion into M−H versus M−R, α and β eliminations.

2.3 Redistribution reactions, fluxional isomerism of allyl, metal carbonyls, cyclopentadienyl and allene systems.

Unit 3: Catalysis by Organometallic Compounds (18 Hrs)

3.1 Homogeneous and heterogeneous organometallic catalysis: Tolman catalytic loops, alkene hydrogenation using Wilkinson catalyst,

3.2 Reactions of carbon monoxide and hydrogen-the water gas shift reaction, synthesis gas based reactions - the Fischer-Tropsch reaction (*synthesis of gasoline*).

3.3 Hydroformylation of olefins using cobalt or rhodium catalyst.

3.4 Polymerization by organometallic initiators and templates for chain propagation - Ziegler Natta catalysts. Polymerisation by metallocene catalysts.

3.5 Carbonylation reactions - Monsanto acetic acid process olefin hydroformylation - oxo process, carbonylation of alkenes and alkynes in the presence of a nucleophile – the Reppe reaction. Carbonylation of aryl halides in the presence of a nucleophile

3.6 Olefin methathesis - synthesis gas based reactions, photodehydrogenation catalyst ("Platinum Pop").

3.7 Oxidation of olefins: Palladium catalysed oxidation of ethylene - the Wacker process, epoxidation of olefins, hydroxylation by metal-oxo complexes

3.8 Asymmetric catalysis - Asymmetric hydrogenation, isomerisation and epoxidation.

3.9 C-H activation and functionalization of alkanes and arenes: Radical type oxidation, hydroxylation, dehydrogenation, carbonylation and regioselective borylation of alkanes and cycloalkanes. Radical type reactions, electrophilic reactions, carbonylation and borylation of arenes. Insertion of alkenes and alkynes in the Ar-H bond.

3.10 Application of palladium catalysts in the formation of C-O and C-N bonds, oxidative coupling reactions of alkynes with other unsaturated fragments for the formation of cyclic and heterocylic compounds. The Dötz reaction.

Unit 4: Bioinorganic Compounds (18 Hrs)

4.1 Essential and trace elements in biological systems, toxic effects of metals (Cd, Hg, Cr and Pb). Mechanism of ion transport across membranes, Sodium-Potassium pump. Ionophores - valinomycin.

4.2 ***Biochemistry of Iron***: Oxygen Carriers- Structure and functions of haemoglobin and myoglobin, Oxygen transport mechanism of Haemoglobin, cooperativity in haemoglobin, Bohr Effect and phosphate effect. Hemerythrin Structure and function.

Redox Metalloenzymes - Cytochromes, Classification, Structure and function, Role in oxidative Phosphorylation of ADP to ATP, Cytochrome P_{450}- Structure and functions. Iron Sulphur Proteins-Rubredoxin, Ferredoxin, Nitrogenase, Structure and function, Nitrogen Fixation. Peroxidases and catalases.

Storage and transport of iron in biological systems-Ferritin, transferrin and Siderophores.

4.3 **Biochemistry of Zinc and Copper**: Structure and functions of carboxypeptidase and carbonicanhydrase, Superoxide dismutase. Structure and functions of various Copper proteins and enzymes. Blue copper proteins (Type-1) - Electron transfer agents - Plastocyanin, Stellacyanin and Azurin. Blue copper Enzymes (Type II) - Ascorbateoxidase, Laccase and ceruloplasmin. Non-Blue copper enzyme (Type III) - Cytochrome oxidase, Amine oxidases, Structure and functions of Hemocyanin.

4.4 Other Important metal containing Biomolecules.

Vitamin B_{12}- Structure and biological importance. Chlorophyll-Photosynthesis, PS I & PS II.

4.5 Metals in medicine - Therapeutic applications of *cis*-platin - Mechanism of action, MRI agents.

Unit 5: Nuclear Chemistry **(9 Hrs)**

5.1 Nuclear Reactions: Q value and reaction threshold, reaction cross section, cross section and reaction rate, neutron capture cross section- variation of neutron capture cross section with energy (1/V law). Nuclear fission - fission fragments and mass distribution, fission yields, fission energy, fission cross section and threshold fission neutrons, nuclear fusion reactions and their applications.

5.2 Principles of counting technique: G.M. counter, proportional, ionization and scintillation counters, cloud chamber.

5.3 Synthesis of transuranic elements: Neptunium, Plutonium, Curium, Berkelium, Einsteinium, Mendelevium, Nobelium, Lawrencium

5.4 Analytical applications of radioisotopes-radiometric titrations, kinetics of exchange reactions, measurement of physical constants including diffusion constants, Radioanalysis, Neutron Activation Analysis, Prompt Gama Neutron Activation Analysis and Neutron Absorptiometry.

5.5 Radiation chemistry of water and aqueous solutions. Measurement of radiation doses. Relevance of radiation chemistry in biology, organic compounds and radiation polymerization.

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SEMESTER I

24P1CHET02: BASIC ORGANIC CHEMISTRY

Credit : 4 **Contact Lecture Hours: 72**

After completing the course, the students will be able to:

	Course Outcome	*POs / PSOs*	*CL*	*KC*	*Class Sessions*
CO1	Explain the basic concepts of organic chemistry.	PO 1 PSO 1	R	F	18
CO2	Illustrate the principles of physical organic chemistry.	PO 1 PSO 1	U	C	9
CO3	Recognize the importance of organic photochemical reactions.	PO 1 PSO 3	U	F	9
CO4	Demonstrate the reactivity and stability of organic molecules based on structure, including conformation and stereochemistry.	PO 1 PSO 4	U	C	36

Unit 1: Basic Concepts in Organic Chemistry (18 Hrs)

1.1 Review of basic concepts in organic chemistry: Bonding, hybridisation, MO theory and MO picture of butadiene, allyl systems and benzene.

1.2 *Electron displacement effects*: Inductive effect, electromeric effect, resonance effect, hyperconjugation, steric effect. Bonding weaker than covalent bonds.

1.3 *Concept of aromaticity*: Delocalization of electrons - Hückel’s rule, criteria for Aromaticity, examples of neutral and charged aromatic systems – annulenes, Azulene, Mesoionic Compounds. Anti-aromatic and homoaromatic systems. NMR as a tool for Aromaticity.

1.4 Mechanism of electrophilic and nucleophilic aromatic substitution reactions with examples. Arenium ion intermediates. S_N1, S_NAr, $S_{RN}1$ and benzyne mechanisms.

1.5 Structure and reactions of α, β- unsaturated carbonyl compounds involving electrophilic and nucleophilic addition - Michael addition, Mannich reaction, Robinson annulation.

Unit 2: Physical Organic Chemistry (9 Hrs)

2.1 Energy profiles. Kinetic versus thermodynamic control of product formation, Hammond postulate, kinetic isotope effects with examples. Linear free energy relationships-Hammet equation, Taft equation.

2.2 HSAB principle and its applications in organic reactions.

2.3 Catalysis by acids, bases and nucleophiles with examples from acetal and cyanohydrin. Ester formation and hydrolysis reactions of esters - $A_{AC}2$, $A_{AC}1$, $A_{AL}1$, $B_{AC}2$ and $B_{AL}1$ mechanisms.

Unit 3: Organic Photochemistry **(9 Hrs)**

3.1 Photoreactions of carbonyl compounds: Norrish reactions of ketones. Patterno - Buchi reaction. Barton (*nitrite ester reaction*); Di-π-methane and Photo Fries rearrangements, photochemistry of conjugated dienes (*butadiene only*), photochemistry of vision.

Unit 4: Stereochemistry of Organic Compounds **(18 Hrs)**

4.1 *Stereoisomerism*: Definition based on symmetry and energy criteria, configuration and conformational stereoisomers, introduction to Akamptisomerism (*basic idea only*)

4.2 *Center of Chirality*: Molecules with C, N, S based chiral centers, absolute configuration, enantiomers, racemic modifications, R and S nomenclature using Cahn-Ingold-Prelog rules, molecules with a chiral center and Cn. molecules with more than one center of chirality, definition of diastereoisomers, constitutionally symmetrical and unsymmetrical chiral molecules, erythro and threo nomenclature.

4.3 Axial, planar and helical chirality with examples, stereochemistry and absolute configuration of allenes, biphenyls and binaphthyls, ansa and cyclophanic compounds, spiranes, exo-cyclic alkylidenecycloalkanes.

4.4 Topicity and prostereoisomerism, topicity of ligands and faces as well as their nomenclature, NMR distinction of enantiotopic/diastereotopic ligands.

4.5 *Geometrical isomerism*: Nomenclature, E-Z notation, methods of determination of geometrical isomers, interconversion of geometrical isomers.

4.6 Significance of stereochemistry in medicinal and agricultural science.

Unit 5: Conformational Analysis **(18 Hrs)**

5.1 *Conformational Descriptors* : Factors affecting conformational stability of molecules, conformational analysis of substituted ethanes, cyclohexane and its derivatives, decalins, adamantane, norbornane, sucrose and lactose.

5.2 Conformation and reactivity of elimination (dehalogenation, dehydrohalogenation, semipinacolic deamination and pyrolytic elimination - Saytzeff and Hofmann eliminations), substitution and oxidation of 2^o alcohols, nucleophilic addition to carbonyl compounds (Cram's rule, Felkin Anh Model)

5.3 Chemical consequence of conformational equilibrium - Curtin Hammett principle.

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1. D. Hellwinkel, *Systematic nomenclature of organic chemistry*, Springer international Edn.
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SEMESTER I

24P1CHET03: PHYSICAL CHEMISTRY - I

Credit : 3 **Contact Lecture Hours: 54**

After completing the course, the students will be able to:

	Course Outcome	*POs / PSOs*	*CL*	*KC*	*Class Sessions*
CO1	Application of mathematical tools to calculate thermodynamic and kinetic properties.	PO 1 PSO 3	A	P	18
CO2	Explain the relationship between microscopic properties of molecules with macroscopic thermodynamic observables.	PO 1 PSO 2	U	C	27
CO3	Explain the kinetic behaviour of gases and their transport properties.	PO 1 PSO 4	U	C	9

Unit 1: Classical Thermodynamics **(12 Hrs)**

1.1 Irreversible processes - Clausius inequality, Thermodynamic equations of State, Maxwell relations and significance. Thermodynamic equations of state. The Nernst Heat Theorem, Third law of thermodynamics – determination of absolute entropies.

1.2 Fugacity, relation between fugacity and pressure, variation of fugacity with temperature and pressure. Activity and activity coefficient.

1.3 Thermodynamics of mixing – Free energy, entropy, enthalpy and volume of mixing, Gibbs-Duhem-Margules equation, applications of Gibbs-Duhem- Margules equation - Konovalov's first and second laws, Henry's law, excess thermodynamic functions-free energy, enthalpy, entropy and volume.

1.4 Chemical affinity and thermodynamic functions, effect of temperature and pressure on chemical equilibrium. Van't Hoff reaction isochore and isotherm. Le Chatelier's Principle – Quantitative treatment.

Unit 2: Phase Equilibrium **(6 Hrs)**

2.1 Three component systems – Phase rule, graphical representation. Solid-liquid equilibria: ternary solutions with common ions, hydrate formation, compound formation.

2.2 Liquid-liquid equilibria – Phase diagrams of systems with one pair of partially miscible liquids, two pairs of partially miscible liquids, three pairs of partially miscible liquids.

Unit 3: Kinetic Theory of Gases **(12 Hrs)**

3.1 Maxwell's law of distribution of velocities - derivation, graphical representation and experimental verification, most probable velocity, derivation of average, RMS and most probable velocities.

3.2 Collision diameter, collision frequency in a single gas and in a mixture of two gases, mean free path, frequency of collision, effusion, the rate of effusion, time dependence of pressure of an effusing gas, the law of corresponding states.

3.3 Transport properties of gases – diffusion, thermal conduction and viscosity of gases.

Unit 4: Statistical Thermodynamics **(18 Hrs)**

4.1 Probability, permutations and combinations, configurations, macrostates and microstates, *equal a priori* principle and thermodynamic probability, ensemble, types of ensembles, phase-space, Stirling's approximation, thermodynamic probability and entropy.

4.2 Boltzmann distribution law, degeneracy, evaluation of β, partition function and its physical significance, canonical partition function and molecular partition function, partition function and thermodynamic functions, separation of molecular partition function - translational, rotational, vibrational, and electronic partition functions. Rotational states of hydrogen, Thermal de-Broglie wavelength.

4.3 Entropy of ideal monoatomic gas - Sackur-Tetrode equation, equilibrium constants and partition function, statistical formulation of third law of thermodynamics, residual entropy.

4.4 *Heat capacity of solids*: The vibrational properties of solids, Dulong and Petit's law, Einstein's theory and its limitations, Debye theory and its limitations.

Unit 5: Quantum Statistics **(6 Hrs)**

5.1 Need for quantum statistics, Bosons and Fermions, *Bose-Einstein statistics*: Bose- Einstein distribution law, Bose-Einstein condensation, first order and higher order phase transitions, liquid helium.

5.2 *Fermi-Dirac statistics*: Fermi-Dirac distribution law, application in electron gas, thermionic emission.

5.3 Comparison of three statistics.

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SEMESTER I

24P1CHET04: QUANTUM CHEMISTRY AND GROUP THEORY

Credit: 4 **Contact Lecture Hours: 72**

	Course Outcome	*POs / PSOs*	*CL*	*KC*	*Class Sessions*
CO1	Explain the fundamentals of group theory.	PO 1 PSO 1	R	F	9
CO2	Apply the principles of group theory in chemical bonding.	PO 1 PSO 3	A	C	27
CO3	Understand the foundation and postulates of quantum mechanics.	PO 1 PSO 3	U	F	6
CO4	Describe the use of simple models for predictive understanding of different molecular systems and phenomena.	PO 1 PSO 4	U	C	21
CO5	Illustrate the concept of atomic orbitals by quantum mechanics.	PO 1 PSO 3	U	C	9

Unit 1: Group Theory and Applications in Chemical Bonding **(36 Hrs)**

1.1 Symmetry elements and symmetry operations.

1.2 Determination of point groups of molecules and ions (organic / inorganic / complex) belonging to C_n, C_s, C_i, C_{nv}, C_{nh}, $C_{\infty v}$, D_{nh}, $D_{\infty h}$, D_{nd}, Td and Oh point groups.

1.3 Symmetry in crystals: 32 crystallographic point groups (*no derivation*), Hermann-Mauguin symbols. Screw axis-pitch and fold of screw axis, glide planes, space groups (*elementary idea only*)

1.4 Mathematical groups: Properties, Abelian groups, cyclic groups, sub groups, similarity transformation, classes – C_{2v}, C_{3v} and C_{2h}.

1.5 Group multiplication tables (GMTs) – C_{2v}, C_{3v} and C_{2h}, isomorphic groups.

1.6 Matrix representation of elements like E, C_n, S_n, I, σ-matrix representation of point groups like C_{2v}, C_{3v}, C_{2h}, C_{4v} – trace /character, block factored matrices.

1.7 Reducible and irreducible representations, standard reduction formula, statement of great orthogonality theorem (GOT). Construction of character tables for C_{2v}, C_{2h}, C_{3v} and C_{4v}.

1.8. Application in chemical bonding: Projection operator, transformation properties of atomic orbitals, construction of symmetry adapted linear combination of atomic orbitals (SALCs) of C_{2v}, C_{3v}, D_{3h} and C_{2h} molecules.

Unit 2: Quantum Mechanics and Applications **(36 Hrs)**

2.1. Experimental foundation of quantum mechanics: Elementary ideas of black body radiation, photoelectric effect and atomic spectra. Need of quantum mechanics. Concept of matter wave, de Broglie relation, uncertainty principle and its consequences. (*Non-evaluative*)

2.2. *Postulates of Quantum Mechanics*:

State function or wave function postulate: Born interpretation of the wave function, well behaved functions, orthonormality of wave functions.

Operator postulate: Operator algebra, linear and nonlinear operators, Laplacian operator, commuting and noncommuting operators, Hermitian operators and their properties, Eigen functions and Eigen values of an operator.

Eigen value postulate: Eigen value equation, Eigen functions of commuting operators.

Expectation value postulate.

*Postulate of time-dependent Schrödinger equation: C*onservative systems and time-independent Schrödinger equation.

2.3. *Translational motion*: Free particle in one-dimension, particle in a one dimensional box with infinite potential walls, particle in a one-dimensional box with finite potential walls-tunneling, particle in a three dimensional box ,separation of variables, degeneracy.

2.4. *Vibrational motion*: One-dimensional harmonic oscillator (complete treatment), Hermite equation (solving by method of power series), Hermite polynomials, recursion relation, wave functions and energies-important features, harmonic oscillator model and molecular vibrations.

2.5. *Rotational motion*: Co-ordinate systems, Cartesian, cylindrical polar and spherical polar coordinates and their relationships. The wave equation in spherical polar coordinates-particle on a ring: the phi equation and its solution, wave functions in the real form. Non-planar rigid rotor (or particle on a sphere): separation of variables, the phi and the theta equations and their solutions, Legendre and associated Legendre equations, Legendre and associated Legendre polynomials. Spherical harmonics (imaginary and real forms), polar diagrams of spherical harmonics.

2.6. *Quantization of angular momentum*: quantum mechanical operators corresponding to angular momenta (L_x, L_y, L_z and L^2), commutation relations between these operators. Spherical harmonics as eigen functions of angular momentum operators L_z and L^2. Ladder operator method for angular momentum, space quantization.

2.7. *Quantum Mechanics of Hydrogen-like Atoms*: Potential energy of hydrogen-like systems. The wave equation in spherical polar coordinates: separation of variables - R, Θ and Φ equations and their solutions, wave functions and energies of hydrogen like atoms. Orbitals: Radial functions, radial distribution functions, angular functions and their plots.

2.8. *Spin orbitals*: Construction of spin orbitals from orbitals and spin functions, spin orbitals for many electron atoms, symmetric and antisymmetric wave functions. Pauli's exclusion principle, slater determinants.

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SEMESTER II

24P2CHET05: INORGANIC CHEMISTRY - II

Credit : 4 **Contact Lecture Hours: 72**

After completing the course, the students will be able to:

	Course Outcome	*POs / PSOs*	*CL*	*KC*	*Class Sessions*
CO1	Understand the structural and bonding aspects of co-ordination compounds.	PO 1 PSO 1	U	F	18
CO2	Explain the spectral and magnetic properties of metal complexes.	PO 1 PSO 3	U	C	18
CO3	Explain the thermodynamic and kinetic aspects of reactions of metal complexes.	PO 1 PSO 1	U	C	18
CO4	Understand the stereochemistry of co-ordination compounds.	PO 1 PSO 1	U	C	9
CO5	Describe the co-ordination chemistry of lanthanoids and actinoids	PO 1 PSO 3	U	F	9

Unit 1: Structural Aspects and Bonding **(18 Hrs)**

1.1 Classification of complexes based on coordination numbers and possible geometries, sigma and pi bonding ligands such as CO, NO, CN-, R_3P, and Ar_3P. Stability of complexes, thermodynamic aspects of complex formation-Irving William order of stability, chelate effect.

1.2 Splitting of d orbitals in octahedral, tetrahedral, square planar, square pyramidal and trigonal bipyramidal fields, LFSE, Dq values, Jahn Teller (JT) effect, theoretical failure of crystal field theory, evidence of covalency in the metal-ligand bond, nephelauxetic effect, ligand field theory, molecular orbital theory - M.O energy level diagrams for octahedral and tetrahedral complexes without and with π- bonding, experimental evidences for pi-bonding.

Unit 2: Spectral and Magnetic Properties of Metal Complexes **(18 Hrs)**

2.1 Electronic Spectra of complexes: Term symbols of d^n system, Racah parameters, splitting of terms in weak and strong octahedral and tetrahedral fields, correlation diagrams for d^1 and d^9 ions in octahedral and tetrahedral fields (*qualitative approach*), d-d transitions, selection rules for electronic transitions-effect of spin orbit coupling and vibronic coupling.

2.2 Interpretation of electronic spectra of complexes: Orgel diagrams and demerits, Tanabe Sugano diagrams, calculation of Dq, B and β (*Nephelauxetic ratio*) values, spectra of complexes with lower symmetries, charge transfer spectra.

2.3 Magnetic properties of complexes-paramagnetic and diamagnetic complexes, molar susceptibility, Gouy method for the determination of magnetic moment of complexes, spin only magnetic moment. Temperature dependence of magnetism- Curie's law, Curie-Weiss law, temperature independent paramagnetism (TIP), spin state cross over, antiferromagnetism-inter and intra molecular interaction, anomalous magnetic moments.

Unit 3: Kinetics and Mechanism of Reactions in Metal Complexes (18 Hrs)

3.1 Thermodynamic and kinetic stability, kinetics and mechanism of nucleophilic substitution reactions in square planar complexes- trans effect-theory and applications, effect of entering ligand, effect of leaving group and effect of ligands already present on reaction rate, effect of solvent and reaction pathways.

3.2 Kinetics and mechanism of octahedral substitution- water exchange, dissociative and associative mechanisms, base hydrolysis, racemization reactions, solvolytic reactions (acidic and basic). Replacement reactions involving multidendate ligands - formation of chelates, effect of H^+ on the rates of substitution of chelate complexes, metal ion assisted and ligand assisted dechelation.

3.3 Electron transfer reactions: Outer sphere mechanism-Marcus theory, Marcus-Hush theory, inner sphere mechanism-Taube mechanism, mixed outer and inner sphere reactions, two electron transfer.

Unit 4: Stereochemistry of Coordination Compounds (9 Hrs)

4.1 Geometrical and optical isomerism in octahedral complexes, resolution of optically active complexes, Principle of ORD and CD, determination of absolute configuration of complexes by ORD and circular dichroism.

4.2 Linkage isomerism: Electronic and steric factors affecting linkage isomerism, symbiosis-hard and soft ligands, Prussian blue and related structures, Macrocycles crown ethers.

Unit 5: Coordination Chemistry of Lanthanoids and Actinoids (9 Hrs)

5.1 Term symbols for lanthanide ions, inorganic compounds and coordination complexes of the lanthanoids upto coordination No.12, electronic spectra and magnetic properties of lanthanoid complexes, organometallic complexes of the lanthanoids - σ-bonded complexes, cyclopentadienyl complexes, organolanthanoid complexes as catalysts. Lanthanide contraction- cause and consequences- Separation of lanthanides by ion exchange and solvent extraction method.

5.2 General characteristics of actinoids-difference between 4f and 5f orbitals, coordination complexes of the actinoids- sandwich complexes, coordination complexes and organometallic compounds of thorium and uranium, comparative account of coordination chemistry of lanthanoids and actinoids with special reference to electronic spectra and magnetic properties.

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SEMESTER II

24P2CHET06: ORGANIC REACTION MECHANISM

Credit : 4 **Contact Lecture Hours: 72**

After completing the course, the students will be able to:

	Course Outcome	*POs / PSOs*	*CL*	*KC*	*Class Sessions*
CO1	Describe the mechanisms of different type's organic reactions.	PO 1 PSO 1	U	F	12
CO2	Explain the chemistry of carbanions, carbocations, carbenes, carbenoids, nitrenes and arynes.	PO 1 PSO 1	U	F	27
CO3	Understand the chemistry of radical reactions and its applications.	PO 1 PSO 1	U	C	9
CO4	Explain the basics and applications of concerted reactions	PO 1 PSO 3	U	C	24

Unit 1: Review of Organic Reaction Mechanisms **(12 Hrs)**

1.1 Review of organic reaction mechanisms with special reference to nucleophilic and electrophilic substitution at aliphatic carbon (S_N^1, S_N^2, SN_i, SE_1 and SE_2) elimination (E1, E2 and E1CB) and addition reactions (Regioselectivity: Markovnikov's addition - carbocation mechanism, anti-Markovnikov's addition - radical mechanism). Elimination *vs* Substitution.

1.2 A comprehensive study on the effect of substrate, reagent, leaving group, solvent, ambident nucleophile and neighbouring group on nucleophilic substitution (SN_1 and SN_2) and elimination (E_1 and E_2) reactions. Stereochemical aspects of elimination reactions.

1.3 Electrophilic substitution *via* enolization and Stork-enamine reaction. Von Ritcher, Vilsmeyer formylation, Jacobson and Gatterman-Koch reactions.

Unit 2: Chemistry of Carbanions **(9 Hrs)**

2.1 *Reactions of carbanions*: C-X bond (X = C, O, N) formations through the intermediary of carbanions. Chemistry of enolates and enamines. Kinetic and Thermodynamic enolates- lithium and boron enolates in aldol Alkylation and acylation of enolates.

2.2 Nucleophilic additions to carbonyls groups. Name reactions under carbanion chemistry – Mechanism of Claisen, Dieckmann, Knoevenagel, Stobbe, Darzen and acyloin condensations, Shapiro reaction and Julia elimination. Favorski rearrangement.

2.3 *Ylides*: Chemistry of Phosphorous and Sulphur ylides - Wittig and related reactions, Peterson olefination.

Unit 3: Chemistry of Carbocations **(9 Hrs)**

3.1 Classical and non-classical carbocations.

3.2 C-X bond (X = C, O, N) formations through the intermediary of carbocations. Molecular rearrangements including Wagner-Meerwein, Pinacol-pinacolone, semi-pinacol, Dienone-phenol and Benzilic acid rearrangements, Noyori annulation, Prins reaction.

3.3 C-C bond formation involving carbocations: Oxymercuration, halolactonisation.

Unit 4: Carbenes, Carbenoids, Nitrenes and Arynes **(9 Hrs)**

4.1 Structure of carbenes (singlet and triplet) - generation of carbenes – Reimer Tiemann reaction, Reactions of carbenes – addition and insertion reactions.

4.2 Rearrangement reactions of carbenes such as Wolff rearrangement - generation and reactions of ylids by carbenoid decomposition.

4.3 Structure, generation and reactions of nitrene and related electron deficient nitrene intermediates.

4.4 Hoffmann, Curtius, Lossen, Schmidt and Beckmann rearrangement reactions.

4.5 Arynes: Generation, structure, stability and reactions. Orientation effect - amination of haloarenes.

Unit 5: Radical Reactions **(9 Hrs)**

5.1 Generation of radical intermediates and their detection using EPR and Magnetic methods. Reactions of radical intermediates - (a) addition to alkenes, alkynes (inter & intramolecular) for C-C bond formation - Baldwin's rules (b) fragmentation and rearrangements – Hydroperoxide: formation, rearrangement and reactions. Auto-oxidation.

5.2 Named reactions involving radical intermediates: Barton deoxygenation and decarboxylation, McMurry coupling.

Unit 6: Concerted reactions **(24 Hrs)**

6.1 Classification: Electrocyclic, sigmatropic, cycloaddition, chelotropic and ene reactions. Woodward Hoffmann rules - frontier orbital and orbital symmetry correlation approaches - PMO method (*for electrocyclic and cycloaddition reactions only*)

6.2 Highlighting pericyclic reactions in organic synthesis such as Claisen, Cope, Wittig, Mislow-Evans and Sommelet-Hauser rearrangements. Diels-Alder and Ene reactions (*with stereochemical aspects*), dipolar cycloaddition (*introductory*).

6.3 Unimolecular pyrolytic elimination reactions: cheletropic elimination, decomposition of cyclic azo compounds, β-eliminations involving cyclic transition states such as N-oxides (Cope reaction), acetates and xanthates (Chugayev reaction)

6.4 Introduction to Click reactions - Mechanism of the Huisgen Azide – Alkyne addition, Mechanism of the 1, 3-Dipolar Cycloaddition, Click reactions, Staudinger ligation and Staudinger reduction.

REFERENCES:

1. R. Bruckner, *Advanced Organic Chemistry: Reaction Mechanism*, Academic Press, 2002.
2. F. A. Carey, R. A. Sundberg, *Advanced Organic Chemistry*, Part B: Reactions and Synthesis, 5^{th} Edn., Springer, New York, 2007.
3. W. Carruthers and I. Coldham, *Modern Methods of Organic Synthesis*, First South Asian Edition, Cambridge University Press, 2005.
4. J. March and M. B. Smith, March's *Advanced Organic Chemistry: Reactions, Mechanisms, and Structure*, 6^{th} Edn., Wiley, 2007.
5. http://www.organic-chemistry.org/namedreactions.
6. R.T. Morrison, R.N. Boyd, S.K. Bhatacharjee, *Organic Chemistry,*7^{th}Edn., Pearson, New Delhi, 2011.
7. J. Clayden, N. Greeves, S.Warren, P.Wothers, *Organic Chemistry*, Oxford University Press, New York, 2004.
8. Fleming, Wiley, *Frontier Orbitals and Organic Chemical Reactions*, London, 1976.
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SEMESTER II

24P2CHET07: PHYSICAL CHEMISTRY - II

Credit: 3 **Contact Lecture Hours: 54**

After completing the course, the students will be able to:

	Course Outcome	*POs / PSOs*	*CL*	*KC*	*Class Sessions*
CO1	Explain the foundations of spectroscopy	PO 1 PSO 2	AN	F	3
CO2	Explain the principles and applications of Microwave, IR, Raman, Electronic and NMR spectroscopy.	PO 1 PSO 1	U	C	42
CO3	Explain EPR, NQR and Mossbauer spectroscopy.	PO 1 PSO 1	U	C	9

Unit 1: Foundations of Spectroscopic Techniques **(3 Hrs)**

Regions of the electromagnetic radiation, origin of spectrum, intensity of absorption, signal to noise ratio, natural line width. Doppler broadening, Lamb dip spectrum, Born Oppenheimer approximation.

Unit 2: Microwave Spectroscopy **(6 Hrs)**

2.1 Principal moments of inertia and classification (linear, symmetric tops, spherical tops and asymmetric tops), selection rules, intensity of rotational lines, relative population of energy levels, derivation of Jmax, effect of isotopic substitution, calculation of intermolecular distance, spectrum of non-rigid rotors.

2.2 Rotational spectra of polyatomic molecules, linear and symmetric top molecules. Stark effect and its application, nuclear spin and electron spin interaction, chemical analysis by microwave spectroscopy.

Unit 3: Infrared and Raman Spectroscopy **(9 Hrs)**

3.1 Morse potential energy diagram, fundamental vibrations, overtones and hot bands, determination of force constants, diatomic vibrating rotator, breakdown of the Born-Oppenheimer approximation, effect of nuclear spin.

3.2 Vibrational spectra of polyatomic molecules, normal modes of vibrations, combination and difference bands, Fermi resonance. FT technique, introduction to FTIR spectroscopy. Instrumentation of FTIR.

3.3 Scattering of light, polarizability and classical theory of Raman spectrum, rotational and vibrational Raman spectrum, complementarities of Raman and IR spectra, mutual exclusion principle, polarized and depolarized Raman lines, resonance Raman scattering and resonance fluorescence.

Unit 4: Electronic Spectroscopy **(9 Hrs)**

4.1 Term symbols of diatomic molecules, electronic spectra of diatomic molecules, selection rules, vibrational coarse structure and rotational fine structure of electronic spectrum. Franck-Condon principle, predissociation, calculation of heat of dissociation, Birge and Sponer method.

4.2 Electronic spectra of polyatomic molecules, spectra of transitions localized in a bond or group, free electron model. Different types of lasers-solid state lasers, continuous wave lasers, gas lasers and chemical laser, frequency doubling, applications of lasers.

Unit 5: Nuclear Magnetic Resonance Spectroscopy **(18 Hrs)**

5.1 NMR spectroscopy: interaction between nuclear spin and applied magnetic field, nuclear energy levels, population of energy levels, Larmor precession, relaxation methods, chemical shift, representation, examples of AB, AX and AMX types, exchange phenomenon, factors influencing coupling, Karplus relationship.

5.2 Second order effects on spectra, spin systems (AB, AB_2), simplification of second order spectra, chemical shift reagents, high field NMR, double irradiation, selective decoupling, NOE effect. Creating NMR signals, effect of pulses, rotating frame reference, FID, FT technique.

5.3 COSY and HETCOR, ^{13}C NMR, natural abundance, sensitivity, ^{13}C chemical shift and structure correlation, ^{19}F, ^{31}P NMR spectroscopy.

Unit 6: Other Magnetic Resonance Techniques **(9 Hrs)**

6.1 EPR Spectroscopy: Electron spin in molecules, interaction with magnetic field, g factor, factors affecting g values, determination of g values ($g_{\parallel}$ and $g_{\perp}$), fine structure and hyperfine structure, Kramers' degeneracy, McConnell equation.

6.2 Theory and important applications of NQR Spectroscopy.

6.3 Mossbauer Spectroscopy: Principle, Doppler effect, recording of spectrum, chemical shift, factors determining chemical shift, application to metal complexes.

REFERENCES:

1. C.N. Banwell, E.M. McCash, *Fundamentals of Molecular Spectroscopy*, 4th Edn. Tata McGraw Hill, 1994.
2. G. Aruldhas, *Molecular Structure and Spectroscopy*, Prentice Hall of India, 2001.
3. A.U. Rahman, M.I. Choudhary, *Solving Problems with NMR Specroscopy*, Academic Press, 1996.
4. D.L. Pavia, G.M. Lampman, G.S. Kriz, *Introduction to Spectroscopy*, 3rd Edn., Brooks Cole, 2000.
5. R.S. Drago, *Physical Methods in Inorganic Chemistry*, Van Nonstrand Reinhold, 1965.
6. R.S. Drago, *Physical Methods in Chemistry*, Saunders College, 1992.
7. W. Kemp, *NMR in chemistry-A Multinuclear Introduction*, McMillan, 1986.
8. H. Kaur, Spectroscopy, 6th Edn., Pragati Prakashan, 2011.
9. H. Gunther, *NMR Spectroscopy*, Wiley, 1995.
10. D.A. McQuarrie, J.D. Simon, *Physical Chemistry: A Molecular Approach*, University Science Books, 1997.
11. D.N. Sathyanarayan, *Electronic Absorption Spectroscopy and Related Techniques*, Universities Press, 2001.
12. D.N. Sathyanarayana, *Vibrational Spectroscopy: Theory and Applications*, New Age International, 2007.
13. D.N. Sathyanarayana, *Introduction To Magnetic Resonance Spectroscopy ESR, NMR, NQR*, IK International, 2009.

SEMESTER II

24P2CHET08: THEORETICAL AND COMPUTATIONAL CHEMISTRY

Credit: 3 **Contact Lecture Hours: 72**

After completing the course, the students will be able to:

	Course Outcome	*Pos / PSOs*	*CL*	*KC*	*Class Sessions*
CO1	Apply the principles of group theory in spectroscopy and hybridization.	PO 1 PSO 3	A	C	12
CO2	Explain the approximation methods in quantum mechanics.	PO 1 PSO 1	U	F	27
CO3	Describe the quantum mechanical explanation of chemical bonding.	PO 1 PSO 1	U	C	9
CO4	Explain the methods of computational quantum chemistry.	PO 1 PSO 3	U	C	24

Unit 1: Application of Group Theory in Spectroscopy **(18 Hrs)**

1.1. Vibrational mode analysis using group theory taking H_2O, NH_3 and *trans*-N_2F_2 as examples using symmetry coordinates and internal coordinates method, prediction of IR and Raman activity, rule of mutual exclusion, redundant modes, out of plane modes.

1.2. Application in UV-visible spectroscopy, selection rules, orbital selection rules, transitions between non-degenerate states, prediction of electronic transitions in C_{2v},C_{3v},C_{4v},C_{2h} and C_{4h} using direct product terms, spin selection rules, relaxation in selection rules and distortion .

1.3. Application in hybridization, determination of hybridization and hybrid functions in CH_4, BF_3 and PCl_5

1.4. Group theory and optical activity (*brief study*)

Unit 2: Approximation Methods in Quantum Mechanics **(18 Hrs)**

2.1 Many-body problem and the need of approximation methods, independent particle model. Variation method: Variation theorem with proof, illustration of variation theorem using the trial function x(a-x) for particle in a 1D-box and using the trial function $e^{-\alpha r}$ for the hydrogen atom, variation treatment for the ground state of helium atom.

2.2 Perturbation method, time-independent perturbation method (*non-degenerate case only*), first order correction to energy and wave function, illustration by application to particle in a 1D-box with slanted bottom, perturbation treatment of the ground state of the helium atom. Qualitative idea of Hellmann-Feynman theorem.

2.3 Hartree-Fock method, multi-electron atoms. Hartree-Fock equations (*no derivation*). The Fock operator, core 43thane43nian, coulomb operator and exchange operator. Qualitative treatment of Hartree-Fock Self-Consistent Field (HFSCF) method. Roothan's concept of basic functions, Slater type orbitals (STO) and Gaussian type orbitals (GTO), sketches of STO and GTO.

Unit 3: Chemical Bonding **(18 Hrs)**

3.1 Schrödinger equation for molecules. Born-Oppenheimer approximation, valence bond (VB) theory, VB theory of H_2 molecule, singlet and triplet state functions (spin orbitals) of H2.

3.2 Molecular Orbital (MO) theory, MO theory of H_2^+ ion, MO theory of H_2 molecule, MO treatment of homonuclear diatomic molecules Li_2, Be_2, N_2, O_2 and F_2 and hetero nuclear diatomic molecules LiH, CO, NO and HF, bond order. Correlation diagrams, non-crossing rule, spectroscopic term symbols for diatomic molecules, comparison of MO and VB theories.

3.3 Hybridization, quantum mechanical treatment of sp, sp2 and sp3 hybridisation. Semiempirical MO treatment of planar conjugated molecules, Hückel Molecular Orbital (HMO) theory of ethene, allyl systems, butadiene and benzene. Calculation of charge distributions, bond orders and free valency.

Unit 4: Computational Quantum Chemistry **(18 Hrs)**

4.1 Introduction and scope of computational chemistry, potential energy surface, conformational search, global minimum, local minima, saddle points.

4.2 *Ab-initio methods*: A review of Hartee-Fock method, self-consistent field (SCF) procedure. Roothan concept basis functions. Basis sets and its classification: Slater type and Gaussian type basis sets, minimal basis set, Pople style basis sets. Hartree-Fock limit. Post Hartree-Fock methods – introduction to Møller-Plesset perturbation theory, configuration interaction, coupled cluster and semi empirical methods.

4.3 *Introduction to Density Functional Theory (DFT) methods*: Hohenberg-Kohn theorems, Kohn-Sham orbitals, exchange correlation functional, local density approximation, generalized gradient approximation, hybrid functionals (*only the basic principles and terms need to be introduced*).

4.4 Comparison of ab-initio, semi empirical and DFT methods.

4.5 *Molecular geometry input*: Cartesian coordinates and internal coordinates, Z-matrix, Z-matrix of single atom, diatomic molecule, non-linear triatomic molecule, linear triatomic molecule, and polyatomic molecules like ammonia, methane and ethane. General format of GAMESS / Firefly input file, single point energy calculation, geometry optimization, constrained optimization and frequency calculation. Koopmans' theorem.

4.6 Features of molecular mechanics force field-bond stretching, angle bending, torsional terms, non-bonded interactions and electrostatic interactions. Commonly used force fields- AMBER and CHARMM.

REFERENCES:

1. N. Levine, *Quantum Chemistry*, 7th Edn., Pearson Education Inc., 2016.
2. P.W. Atkins, R.S. Friedman, *Molecular Quantum Mechanics*, 4th Edn., Oxford University Press, 2005.
3. D.A. McQuarrie, *Quantum Chemistry*, University Science Books, 2008.
4. J.P. Lowe, K Peterson, *Quantum Chemistry*, 3rd Edn., Academic Press, 2006.
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6. R.K. Prasad, *Quantum Chemistry*, 3rd Edn., New Age International, 2006.
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8. H. Metiu, *Physical Chemistry: Quantum Mechanics*, Taylor & Francis, 2006.
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10. M.S. Pathania, *Quantum Chemistry and Spectroscopy (Problems & Solutions)*, Vishal Publications, 1984.
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12. L. H. Hall, *Group Theory and Symmetry in Chemistry*, McGraw Hill, 1969.
13. V. Ramakrishnan, M.S. Gopinathan, *Group Theory in Chemistry*, Vishal Publications, 1992.
14. S. Swarnalakshmi, T. Saroja, R.M. Ezhilarasi, *A Simple Approach to Group Theory in Chemistry*, Universities Press, 2008.
15. S.F.A. Kettle, *Symmetry and Structure: Readable Group Theory for Chemists*, 3rd Edn., Wiley, 2007.
16. A. Vincent, *Molecular Symmetry and Group Theory: A Programmed Introduction to Chemical Applications*, 2nd Edn., Wiley, 2000.
17. A.S. Kunju, G. Krishnan, *Group Theory and its Applications in Chemistry*, PHI Learning, 2010.
18. K.I. Ramachandran, G. Deepa, K. Namboori, *Computational Chemistry and Molecular Modeling: Principles and Applications*, Springer, 2008.
19. A. Hinchliffe, *Molecular Modelling for Beginners*, 2nd Edn., John Wiley & Sons, 2008.
20. C.J. Cramer, *Essentials of Computational Chemistry: Theories and Models*, 2nd Edn., John Wiley & Sons, 2004.
21. D.C. Young, *Computational Chemistry: A Practical Guide for Applying Techniques to Real World Problems*, John Wiley & Sons, 2001.

Softwares:

A) Molecular Mechanics: Arguslab, Tinker, NAMD, DL-POLY, CHARMM, AMBER

B) Ab initio, semiempirical and DFT:

1. Firefly / PC GAMESS available from http://classic.chem.msu.su/gran/gamess/
2. WINGAMESS available from http://www.msg.ameslab.gov/gamess/

C) Graphical User Interface (GUI):

1. Gabedit available from http://gabedit.sourceforge.net/
2. wxMacMolPlt available from http://www.scl.ameslab.gov/MacMolPlt

SEMESTERS I & II

24P2CHEP01: INORGANIC CHEMISTRY PRACTICAL-I

Credit: 3 **Contact Lab Hours: 54+54=108**

After completing the course, the students will be able to:

	Course Outcome	***Pos / PSOs***	***CL***	***KC***	***Class Sessions***
CO1	Illustrate the separation and identification of mixture of cations.	PO 1 PSO 5	A	P	54
CO2	Perform colorimetric estimations.	PO 1 PSO 5	A	P	27
CO3	Prepare and characterize coordination compounds.	PO 1 PSO 5	A	P	27

PART I

Separation and identification of a mixture of four cations (a mixture of two familiar ions such as Ag^{+}, Hg^{2+}, Pb^{2+}, Cu^{2+}, Bi^{2+}, Cd^{2+}, As^{3+}, Sn^{2+}, Sb^{3+}, Fe^{2+}, Fe^{3+}, Al^{3+}, Cr^{3+}, Zn^{2+} , Mn^{2+}, Co^{2+}, Ni^{2+}, Ca^{2+}, Sr^{2+}, Ba^{2+}, Mg^{2+}, Li^{+} , Na^{+} , K^{+} and NH_4^{+} and two less familiar metal ions such as Tl, W, Se, Mo, Ce, Th, Ti, Zr, V, U and Li).

Anions which need elimination not to be given. Minimum eight mixtures to be given.

PART II

Colorimetric estimation of Fe, Cu, Ni, Mn, Cr, and NH_4^{+}, nitrate and phosphate ions.

PART III

Preparation and characterization complexes using IR, NMR and electronic spectra.

(a) Tris (thiourea)copper(I) complex

(b) Potassium tris (oxalate) aluminate (III).

I Hexammine cobalt (III) chloride.

(d) Tetrammine copper (II) sulphate.

I Schiff base complexes of various divalent metal ions.

(f) Bis(dimethylglyoximato)nickel(II)

(g) Prussian blue

REFERENCES:

1. A.I. Vogel, G. Svehla, Vogel's Qualitative Inorganic Analysis, 7th Edn. Longman, 1996.
2. A.I. Vogel, A Text Book of Quantitative Inorganic Analysis, Longman, 1966.
3. I.M. Koltoff, E.B. Sandell, Text Book of Quantitative Inorganic analysis, 3rd Edn. McMillian, 1968.
4. V.V. Ramanujam, Inorganic Semimicro Qualitative Analysis, The National Pub. Co., 1974.
5. J. Singh, R. K. P. Singh, J. Singh, LDS Yadav, I. R. Siddiqui, J. Shrivastava, Advanced Practical Chemistry, Pragati Prakashan, and 7th Edn. 2017.

SEMESTERS I & II

24P2CHEP02: ORGANIC CHEMISTRY PRACTICAL – I

CREDIT: 3 **Contact Lab Hours: 54+54=108**

After completing the course, the students will be able to:

	Course Outcome	***Pos / PSOs***	***CL***	***KC***	***Class Sessions***
CO1	Carry out different methods of separation and purification of organic compounds.	PO 1 PSO 5	A	P	54
CO2	Apply the methods of separation and purification to organic binary mixtures.	PO 1 PSO 5	A	P	27
CO3	Construct the organic structures and reaction schemes using ChemSketch.	PO 1 PSO 5	A	P	27

PART I

General methods of separation and purification of organic compounds such as:

1. Solvent extraction.
2. Soxhlet extraction of a natural product from its source.
3. Fractional crystallization.
4. TLC and Paper Chromatography.
5. Column Chromatography.
6. Membrane Dialysis.

PART II

1. Separation of Organic binary mixtures by chemical/physical separation methods.
2. Purification of organic compounds by column chromatography.
3. Record the IR spectrum of simple organic compounds and Identification of the functional groups.

PART III

Drawing the structures of organic molecules and reaction schemes by Chemsketch.

1. Cycloaddition of diene and dienophile (Diels-Alder reaction)
2. Oxidation of primary alcohol to aldehyde and then to acid
3. Benzoin condensation
4. Esterification of simple carboxylic acids
5. Aldol condensation

REFERENCES:

1. A.I.Vogel, *A Textbook of Practical Organic Chemistry, Longman*, 1989.
2. A.I.Vogel, *Elementary Practical Organic Chemistry*, Longman, 1957.
3. F.G.Mann and B.C Saunders, *Practical Organic Chemistry*, 2009.
4. J. R.Johnson, J.F.Wilcox, *Laboratory Experiments in Organic Chemistry*, Macmillan, 1979.

SEMESTERS I & II

24P2CHEP03: PHYSICAL CHEMISTRY PRACTICAL-I

Credit: 3 **Contact Lab Hours: 72+72 =144**

(One question each from both parts A and B will be asked for the examination)

After completing the course, the students will be able to:

	Course Outcome	***Pos / PSOs***	***CL***	***KC***	***Class Sessions***
CO1	Illustrate experiments related to adsorption, phase diagrams, distribution law and surface tension.	PO 1 PSO 5	A	P	100
CO2	Apply the methods of computational chemistry to solve different problems of chemistry.	PO 1 PSO 5	A	P	44

<u>Part A</u>

I. Adsorption

1. Verification of Freundlich and Langmuir adsorption isotherm: charcoal-acetic acid or charcoal-oxalic acid system.
2. Determination of the concentration of the given acid using the isotherms.

II. Phase diagrams

1. Construction of phase diagrams of simple eutectics.
2. Effect of (KCl / succinic acid) on miscibility temperature.
3. Construction of phase diagrams of three component systems with one pair of partially miscible liquids.

III. Distribution law

1. Distribution coefficient of iodine between an organic solvent and water.
2. Distribution coefficient of benzoic acid between benzene and water.
3. Determination of the equilibrium constant of the reaction $KI + I_2 \leftrightarrow KI_3$

IV. Surface tension

1. Determination of the surface tension of a liquid by:

   a) Drop number method b) Drop weight method

2. Determination of the composition of two liquids by surface tension measurements
3. To determine the critical Micelle concentration of sodium lauryl sulphate

4. Determine the surface excess of amyl alcohol.

V Viscosity

1. Determination of viscosity of pure liquids.
2. Determination of the composition of binary liquid mixtures (alcohol-water, Toluene-nitrobenzene) and verification of Kendall's equation
3. Determination of the molecular weight of a polymer (polystyrene in toluene).
4. Determine the concentration of the given solution of Glycerol/sucrose.

References

01. J.B. Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, 2001.

02. G.W. Garland, J.W. Nibler, D.P. Shoemaker, Experiments in Physical Chemistry, 8th Edn. McGraw Hill, 2009.

03. B. Viswanathan, Practical Physical chemistry, Viva Pub., 2005

04. Saroj Kumar and Naba Kumar, Physical Chemistry Practical, New Central Book Agency, 2012.

05. Practical Physical Chemistry Paperback, 1974 by A.M. James, F.E. Prichard.

<u>Part B</u>

List of Computational Chemistry Experiments

(Second Module of Physical Chemistry Practical –I)

(*These experiments are related to the topics in organic chemistry and physical chemistry covered in BSc-MSc Chemistry courses. From the list of experiments we can select the performable experiments depend on the availability of time and suitable computational chemistry software*)

1. Geometry optimization and single point energy calculations of simple organic molecules
2. Calculation of energy gap between HOMO and LUMO in simple molecules and visualization of molecular orbitals
3. Calculation of dipole moment in polar organic molecules.
4. Calculation of electrostatic charges of atoms in organic molecules using population analysis
5. Calculation of Resonance energy of aromatic compounds
6. Prediction of the stability of *ortho*, *meta*, *para* products of nitration of aromatic ring using computational chemistry calculations.
7. Calculation of IR stretching frequencies of groups and visualization of normal modes of vibration in organic molecules.
8. Calculation of dimerization energy of carboxylic acids
9. Perform the conformational analysis of butane using potential energy scan
10. Find the transition state of simple organic reactions and plot the reaction profile.

11. Determination of heat of hydration of organic molecules.
12. Find the Gibbs free energy of simple gaseous phase reactions and calculate equilibrium constant.
13. Spectral analysis (UV, IR and NMR) of simple organic molecules.
14. Perform molecular dynamic simulations of smaller molecules in water.
15. Calculation of Pk_a of simple organic molecules and compare it with experimental values
16. Docking studies involving protein ligand interactions.
17. Calculation of electrophilicity index in hard-soft acids and bases.

REFERENCES:

1. J. Foresman & Aelieen Frisch, *Exploring Chemistry with Electronic Structure Methods*, Gaussian Inc., 2000.
2. D.C. Young, Computational Chemistry: A Practical Guide for Applying Techniques to Real-World Problems, John Wiley & Sons, 2001.
3. D. Rogers *Computational Chemistry Using the PC, 3rd Edition*, John Wiley & Sons (2003).
4. A. Leach, Molecular Modelling: Principles and Applications, 2nd Edn, Longman, 2001.
5. J. M. Haile (2001) *Molecular Dynamics Simulation: Elementary Methods*.

SEMESTER III

24P3CHET09: INORGANIC CHEMISTRY – III

Credit: 4 **Contact Lecture Hours: 72**

After completing the course, the students will be able to:

	Course Outcome	*Pos / PSOs*	*CL*	*KC*	*Class Sessions*
CO1	Describe the structure, reactions and phase transitions of solid state	PO 1 PSO 1	U	F	18
CO2	Explain the electrical, magnetic and optical properties of solids.	PO 1 PSO 1	R	F	18
CO3	Explain the structure and applications of inorganic chains, rings, cages and clusters, and organometallic polymers.	PO 1 PSO 3	A	C	27
CO4	Describe the synthesis of solids and applications of magnetonano particles.	PO 1 PSO 3	U	C	9

Unit 1: Solid State Chemistry **(18 Hrs)**

1.1 *Structure of solids*: Structure of compounds of AX (Zinc blende, Wurtzite), AX_2 (Rutile, fluorite, antifluorite), ABX_3 (Perosvskite, Ilmenite). Spinels. Inverse spinel structures.

1.2 Diffusion in solids. Mechanisms- vacancy diffusion, interstitial diffusion, Interstitialcy diffusion, Ring mechanism. Diffusion equation- Coefficient of diffusion atomic approach.

1.3 Solid state reactions-Factors affecting the rate of solid state reactions- Reaction condition, Structural factor, Nucleation and growth, Surface area of solids, Surface structure and reactivity, Wagner reaction mechanism, Kirkendall effect. Thermal decomposition of solids: Type I and Type II reactions.

1.4 Phase transition in solids- Buerger's Classification of phase transitions, Reconstructive and Displacive Transitions. Thermodynamic Classification-first and second order phase transitions (Brief study only). Nucleation, growth and critical size in phase transition. Order-disorder transitions and Martensitic transformations.

1.5 Crystal Growth. Growth of Single crystal. Various Techniques-Crystal growth from melt-Czohralski method, Bridgman and Stockbarger method, Zone melting. Crystallization from solution-Hydro thermal method, gel method. Crystal growth from Vapour- Chemical Vapour Deposition.

1.6 Solid Electrolytes- Solid cationic electrolytes, Solid anionic electrolytes, Mixed ionic electronic conductors.

1.7 Solid solution-Substitutional Solid Solution, Requirements for formation, Interstitial Solid Solution, Metal alloys, Engel-Brewer rule, Intermetallic compounds, Hume-Rothery Compounds, Zintal Phase.

Unit 2: Electrical, Magnetic and Optical Properties of Solids (18 Hrs)

2.1 Free electron theory of solids. Zone theory of solids (*quantum mechanical approach*). Energy bands-conductors and non-conductors, Mechanism of intrinsic and extrinsic semiconductors. Mobility of charge carriers- Hall Effect (*derivation required*). Piezo electricity, pyroelectricity and ferro electricity- hysteresis.

2.2 Magnetic properties of transition metal oxides, garnets, spinels, ilmenites and perovskites, magnetoplumbites. Photoconductivity, photovoltaic effects, luminescence, applications of optical properties-phosphors, solid state lasers and solar cells.

2.3 Conductivity of pure metals. Super conductivity-Type I and Type II superconductors, Meisner effect, BCS theory of superconductivity (*derivation not required*)-Cooper pairs. High temperature superconductors, super conducting cuprates – YbaCu oxide system. Josephson's Junction, conventional superconductors, organic superconductors, fullerenes.

Unit 3: Inorganic Chains and Rings (9 Hrs)

3.1 *Chains*: Catenation, heterocatenation, Silicones, Silicates, and Zeolites: Synthesis, structure and applications, isopoly acids of vanadium, molybdenum and tungsten, heteropoly acids of Mo and W.

3.2 *Rings*: Topological approach to boron hydrides, styx numbers. Heterocyclic inorganic ring systems: Structure and bonding in phosphorous-sulphur, phosphorous-nitrogen and sulphur-nitrogen compounds, polythiazil. ^{31}P nmr spectrum of phosphorus – sulphur and phosphorous-nitrogen compounds. Homocyclic inorganic ring systems: Structure and bonding in sulphur, selenium.

Unit 4: Inorganic Cages and Clusters (9 Hrs)

4.1 Synthesis, structure and bonding of cage like structures of phosphorous. Boron cage Aluminium, indium and gallium clusters, cages and clusters of germanium, tin and lead, cages and clusters of tellurium, Mercuride clusters in amalgams. Medical applications of boron clusters- nucleic acid precursors, DNA binders, application of C_2B_{10} for Drug Design, Nuclear receptor ligands bearing C_2B_{10} cages.

Unit 5: Organometallic Polymers (9 Hrs)

5.1 Polymers with organometallic moieties as pendant groups, polymers with organometallic moieties in the main chain, condensation polymers based on ferrocene and on rigid rod polyynes, poly(ferrocenylsilane)s, applications of Poly(ferrocenylsilane)s and related polymers, applications of rigid-rod polyynes, polygermanes and polystannanes, polymers prepared by ring opening polymerization, organometallic dendrimers.

Unit 6: Synthesis of Solids and Magnetic Nanoparticles (9 Hrs)

6.1 *Synthesis of Solids*: Nucleation, growth, epitaxy and topotaxy, methods for the synthesis of $MgAl_2O_4$, silica glass, indium tin oxide and their coatings, zeolites and alumina based abrasives, hydrothermal synthesis, intercalation and deintercalation, preparation of thin films, electrochemical methods, chemical vapour deposition. Synthesis of amorphous silica and diamond films, sputtering and laser ablation.

6.2 Magnetic nanoparticles, superparamagnetism and thin films, applications of magnetic nanoparticles – data storage, Magnetic Resonance Imaging (MRI) and Contrast Enhancement using magnetic nanoparticles, biomedical applications of magnetic nanoparticles.

REFERENCES:

1. L.V. Azaroff, *Introduction to Solids*, Mc Graw Hill, 1984.
2. A.R. West, *Solid State Chemistry and its Applications*, Wiley-India, 2007.
3. D.K. Chakrabarty, *Solid State Chemistry*, New Age Pub., 2010.
4. D.M. Adams, *Inorganic Solids: An Introduction to Concepts in Solid State Structural Chemistry*, Wiley, 1974.
5. C.N.R. Rao, K.J. Rao, *Phase Transitions in Solids*, McGraw Hill, 2010.
6. B.E. Douglas, D.H. McDaniel, J.J. Alexander, *Concepts and Models of Inorganic Chemistry*, 3rd Edn., John Wiley & sons, 2006.
7. A. Earnshaw, *Introduction to Magnetochemistry*, Academic Press, 1968.
8. J.E. Huheey, E.A. Keiter, R.L. Keiter, *Inorganic Chemistry Principles of Structure and Reactivity*, 4th Edn., Harper Collins College Pub.,1993.
9. F.A. Cotton, G. Wilkinson, C.A. Murillo, M. Bochmann, *Advanced Inorganic Chemistry*, 6th Edn., Wiley-Interscience,1999.
10. K.F. Purcell, J.C. Kotz, *Inorganic Chemistry*, Holt-Saunders, 1977.
11. Wai Kee Li, Gong-Du Zhou, Thomas Chung Wai Mak, *Advanced Structural Inorganic Chemistry*, International Union of Crystallography, 2008.
12. Matthias Driess, Heinrich Nöth, *Molecular Clusters of the Main Group Elements*, Wiley-VCH, 2004.
13. Richard J.D. Tilley, *Understanding Solids*, 2nd edition, Wiley, 2013.
14. G.L. Hornyak, J.J. Moore, H.F. Tibbals, J. Dutta, *Fundamentals of Nanotechnology*, CRC Press, 2009.
15. Chris Binns, *Introduction to Nanoscience and Nanotechnology*, Wiley, 2010.
16. Vadapalli Chandrasekhar, *Inorganic and Organometallic Polymers*, Springer, 2005.
17. Anthony R. West, *Basic Solid State Chemistry*, John Wiley and Sons, 1988.

SEMESTER III

24P3CHET10: ORGANIC SYNTHESES

Credit: 4 **Contact Lecture Hours: 72**

After completing the course, the students will be able to:

	Course Outcome	*Pos / PSOs*	*CL*	*KC*	*Class Sessions*
CO1	Describe the applications of oxidation and reduction techniques in organic syntheses.	PO 1 PSO 2	A	C	18
CO2	Illustrate modern synthetic methods and applications of reagents.	PO 1 PSO 1	U	C	15
CO3	Explain different methods for the construction of carbocyclic and heterocyclic ring systems.	PO 1 PSO 3	U	F	12
CO4	Understand the principles and applications of protecting groups in chemistry.	PO 1 PSO 3	U	C	9
CO5	Apply retrosynthetic analysis to design the synthesis of a target molecule.	PO 1 PSO 3	U	C	9
CO6	Understand the principles and applications of supramolecular chemistry.	PO 1 PSO 3	A	C	9

Unit 1: Organic Synthesis *via* Oxidation and Reduction **(18 Hrs)**

1.1 Survey of organic reagents and reactions in organic chemistry with special reference to oxidation and reduction. Metal based and non-metal based oxidations of (a) alcohols to carbonyls (Chromium, Manganese, aluminium and DMSO based reagents). (b) Alkenes to epoxides (peroxides/per acids based) - Sharpless asymmetric epoxidation, Jacobsen epoxidation, Shi epoxidation. (c) Alkenes to diols (Manganese and Osmium based) - Prevost reaction and Woodward modification (d) alkenes to carbonyls with bond cleavage (Manganese and lead based, ozonolysis) (e) alkenes to alcohols/carbonyls without bond cleavage-hydroboration-oxidation, Wacker oxidation, selenium, chromium based allylic oxidation (f) ketones to ester/lactones- Baeyer-Villiger.

1.2 (a) Catalytic hydrogenation (Heterogeneous: Palladium/Platinum/Rhodium and Nickel. Homogeneous: Wilkinson).(b) Metal based reductions- Birch reduction, pinacol formation, acyloin formation (c) Hydride transfer reagents from Group III and Group IV in reductions - $LiAlH_4$, DIBAL-H, Red-Al, $NaBH_4$ and $NaCNBH_3$, Selectrides, trialkylsilanes and trialkylstannane, Meerwein-Pondorff-Verley reduction.

Unit 2: Modern Synthetic Methods and Reagents **(15 Hrs)**

2.1 Baylis-Hillman reaction, Henry reaction, Nef reaction, Ritter reaction, Sakurai reaction, Multicomponent reactions – Passerini reactions and Ugi reaction, Brook rearrangement, Tebbe olefination. Metal mediated C-C and C-X coupling reactions: Heck, Stille, Suzuki, Negishi and Sonogashira reactions, Nozaki-Hiyama, Buchwald-Hartwig, Ullmann and Glaser coupling reactions. Wohl-Ziegler reaction. Mitsunobu reaction, Reformatsky reactions.

2.2 Reagents such as: NBS, DDQ, DCC. Gilmann reagent.

2.3 Native chemical ligation

Unit 3: Construction of Carbocyclic and Heterocyclic Ring Systems (9 Hrs)

3.1 The synthesis of four, five and six-membered rings- ketene cycloaddition (inter- and intramolecular)- Pauson-Khand reaction, Volhardt reaction, Bergman cyclization, Nazarov cyclization, radical cyclization.

3.2 Inter-conversion of ring systems (contraction and expansion)-Demjenov reaction, Construction of macrocyclic rings - ring closing metathesis.

3.3 Formation of heterocyclic rings: Preparation and structure of the following heterocyclics- azeridine, oxirane, thirane, oxaziridine, azetidine and thietane, 5-membered ring heterocyclic compounds with one or more than 1 hetero atom like N, S or O- Pyrrole, furan, thiophene, imidazole, thiazole and oxazole.

Unit 4: Protecting Group Chemistry (9 Hrs)

4.1 Protection and deprotection of hydroxy, carboxyl, carbonyl, and amino groups. Chemo- and regioselective protection and deprotection. Illustration of protection and deprotection in synthesis.

4.2 Protection and deprotection in peptide synthesis: Common protecting groups used in peptide synthesis- Protecting groups used in solution phase and solid phase peptide synthesis (SPPS).

4.3 Role of trialkyl silyl group in organic synthesis.

Unit 5: Retrosynthetic Analysis (12 Hrs)

5.1 Basic principles and terminology of retrosynthesis: synthesis of aromatic compounds, one group and two group C-X disconnections; one group C-C and two group C-C disconnections.

5.2 Amine and alkene synthesis: important strategies of retrosynthesis, functional group transposition, important functional group interconversions. Retrosynthesis of luciferin. Functional equivalents and reactivity - Umpolung reaction (*Ireland-Claisen rearrangement*).

Unit 6: Molecular Recognition and Supramolecular Chemistry (9 Hrs)

6.1 Concept of molecular recognition- host-guest complex formation- Forces involved in molecular recognition.

6.2 Molecular receptors: Cyclodextrins, crown ethers, cryptands, spherands, tweezers, carcerands, cyclophanes, calixarenes.

6.3 Importance of molecular recognition in nucleic acids and protein.

6.4 Applications of supramolecular complexes in medicine- targeted drug delivery.

REFERENCES:

1. M.B. Smith, *Organic Synthesis*, 3rd Edn.,Wave function Inc., 2010.
2. F.A. Carey, R. I. Sundberg, *Advanced Organic Chemistry*, Part A and B, 5th Edn. Springer, 2007.
3. S. Warren, P. Wyatt, *Organic Synthesis: The Disconnection Approach*, 2nd Edn. Wiley, 2008.
4. www.arkat-usa.org (Retrosynthesis of D-luciferin).
5. I. Ojima, *Catalytic Asymmetric Synthesis*, 3rd Edn., John Wiley & Sons, 2010.
6. W. Carruthers, I. Coldham, *Modern Methods of Organic Synthesis*, 4th Edn. Cambridge University Press, 2004.
7. J. Clayden, N. Greeves, S. Warren, P. Wothers, *Organic Chemistry*, Oxford University Press, 2001.
8. R. Noyori, *Asymmetric Catalysis in Organic Synthesis*, John Wiley & Sons, 1994.
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10. R.O.C. Norman, J. M. Coxon, *Principles of Organic Synthesis*, 3rd Edn., Chapmann and Hall, 1993.
11. V. K. Ahluwalia, L. S. Kumar, S. Kumar, *Chemistry of Natural Products*, CRS Press, 2007.
12. J.M. Lehn, *Supramolecular Chemistry*: Concepts and Perspectives, VCH, 1995.

SEMESTER III

24P3CHET11: PHYSICAL CHEMISTRY - III

Credit: 4 **Contact Lecture Hours: 72**

After completing the course, the students will be able to:

	Course Outcome	***POs / PSOs***	***CL***	***KC***	***Class Sessions***
CO1	Apply the principles of chemical kinetics in different types of reactions.	PO 1 PSO 3	U	C	27
CO2	Describe the chemistry of surfaces and its applications in colloids and macromolecules.	PO 1 PSO 1	U	F	27
CO3	Explain the chemistry of crystalline solids	PO 1 PSO 1	U	F	18

Unit 1: Chemical Kinetics - I **(9Hrs)**

a. *Theories of reaction rates*: Collision theory, kinetic theory of collisions, steric factor potential energy surfaces. Conventional transition state theory, thermodynamic formulation of the reaction rate-Eyring equation. Comparison of the two theories. Significance of $\Delta G^{\neq}$, $\Delta H^{\neq}$ and $\Delta S^{\neq}$, volume of activation. Effect of pressure and volume on velocity of gas reactions.

b. Enzyme catalysis and its mechanism, Michelis-Menten equation, effect of pH and temperature on enzyme catalysis.

Unit 2: Chemical Kinetics - II **(18 Hrs)**

2.1 *Unimolecular reactions*: Lindemann - Hinshelwood mechanism, qualitative idea of RRKM theory.

2.2 *Chain reactions*: Chain initiation processes, steady state treatment, kinetics of H_2-Cl_2 and H_2-Br_2 reactions, Rice-Herzfeld mechanism for decomposition of ethane and acetaldehyde, Goldfingr-Letort-Niclause rules, branching chains, Semenov- Hinshelwood mechanism of branching chains, upper and lower explosion limits, the H_2-O_2 reaction,

2.3 *Fast reactions*: Relaxation, flow and shock methods, flash photolysis, NMR and ESR methods of studying fast reactions.

2.4 *Reactions in solution*: Factors determining reaction rates in solutions, effect of dielectric constant and ionic strength, cage effect, Bronsted-Bjerrum equation, primary and secondary kinetic salt effect.

2.5 *Acid-base catalysis*: Specific and general catalysis, Skrabal diagram, Bronsted catalysis law, prototropic and protolytic mechanism with examples, acidity function.

Unit 3: Surface Chemistry (18 Hrs)

3.1 Different types of surfaces, thermodynamics of surfaces, Gibbs adsorption equation and its verification, surfactants and micelles, surface films, surface pressure and surface potential and their measurements and interpretation.

3.2 Application of low energy electron diffraction and photoelectron spectroscopy, ESCA and Auger electron spectroscopy, scanning probe microscopy-AFM and STM, ion scattering, SEM and TEM in the study of surfaces.

3.3 Surface Enhanced Raman scattering, surfaces for SERS studies, chemical enhancement mechanism, principle and application of SERS in surface chemistry.

3.4 *Adsorption*: The Langmuir theory, kinetic and statistical derivation, multilayer adsorption-BET theory, Use of Langmuir and BET isotherms for surface area determination. Application of Langmuir adsorption isotherm in surface catalysed reactions, the Eley-Rideal mechanism and the Langmuir-Hinshelwood mechanism, flash desorption.

Unit 4: Colloids and Macromolecules (9 Hrs)

4.1 *Colloids*: Structure and stability, the electrical double layer, zeta potential, electrokinetic phenomena - sedimentation potential and streaming potential, Donnan membrane equilibrium.

4.1 *Macromolecules*: Different averages, methods of molecular mass determination - osmotic, viscosity, sedimentation and light scattering methods.

Unit 5: Electrochemistry - I (18 Hrs)

5.1 Theories of ions in solution, Drude and Nernst's electrostriction model and Born's model, Debye-Huckel theory, derivation of Debye-Huckel-Onsager equation, validity of DHO equation for aqueous and non-aqueous solutions, Debye-Falkenhagen effect, conductance with high potential gradients, activity and activity coefficients in electrolytic solutions, ionic strength, Debye-Huckel limiting law and its various forms, qualitative and quantitative tests of Debye-Huckel limiting equation, deviations from the DHLL, ion association, triple ions and conductance minima.

REFERENCES:

1. J. Rajaram, J.C. Kuriakose, *Kinetics and Mechanisms of Chemical Transformations*, Macmillan India, 2000.
2. K.J. Laidler, *Chemical kinetics*, 3rd Edn., Harper & Row, 1987.
3. C. Kalidas, *Chemical Kinetic Methods: Principles of Fast Reaction Techniques and Applications*, New Age International, 2005.
4. J.W. Moore, R.G. Pearson, *Kinetics and Mechanisms*, John Wiley & Sons, 1981.
5. P.W. Atkins, *Physical Chemistry*, 9th Edn, Oxford University press, 2010
6. D.A. McQuarrie, J.D. Simon, *Physical chemistry: A Molecular Approach*, University Science Books, 1997
7. A.W. Adamson, A.P. Gast, *Physical Chemistry of Surfaces*, 6th Edn., John Wiley & sons, 1997.
8. L.V. Azaroff, *Introduction to Solids*, Mc Graw Hill, 1984.
9. D. K. Chakrabarty, *Solid State Chemistry*, New Age Pub., 2010.
10. A. R. West, *Basic Solid State Chemistry*, John Wiley & Sons, 1999.

SEMESTER III

24P3CHET12: SPECTROSCOPIC METHODS IN CHEMISTRY

Credit: 3 **Contact Lecture Hours: 54**

After completing the course, the students will be able to:

	Course Outcome	*POs / PSOs*	*CL*	*KC*	*Class Sessions*
CO1	Describe the principles of UV-visible, Chiro-optical, IR, NMR and Mass spectroscopic techniques.	PO 1 PSO 1	U	C	20
CO2	Illustrate various spectroscopic techniques using simple problems.	PO 1 PSO 4	A	C	25
CO3	Elucidate the structure of an unknown organic compound using data from various spectroscopic techniques.	PO 1 PSO 3	U	C	9

Unit 1: Ultraviolet-Visible and Chiro-optical Spectroscopy **(9 Hrs)**

1.1 Energy levels and selection rules, Woodward-Fieser and Fieser-Kuhn rules.

1.2 Influence of substituent, ring size and strain on spectral characteristics. Solvent effect and Stereochemical effect. Chiro-optical properties - ORD, CD, octant rule, axial haloketone rule, Cotton effect-applications.

1.3 Problems based on the above topics.

Unit 2: Infrared Spectroscopy **(9 Hrs)**

2.1 Fundamental vibrations, characteristic regions of the spectrum (fingerprint and functional group regions), influence of substituent, ring size, hydrogen bonding, vibrational coupling and field effect on frequency, determination of stereochemistry by IR technique.

2.2 IR spectra of C=C bonds (olefins and arenes) and C=O bonds.

2.3 Problems on spectral interpretation with examples.

Unit 3: Nuclear Magnetic Resonance Spectroscopy **(18 Hrs)**

3.1 Magnetic nuclei with special reference to ^{1}H and ^{13}C nuclei. Chemical shift and shielding/deshielding, factors affecting chemical shift, relaxation processes, chemical and magnetic non-equivalence, local diamagnetic shielding and magnetic anisotropy. ^{1}H and ^{13}C NMR scales.

3.2 Spin-spin splitting: AX, AX_2, AX_3, A_2X_3, AB, ABC, AMX type coupling, homonuclear/heteronuclear couplings, first order and non-first order spectra, Pascal's triangle, coupling constant, mechanism of coupling- Dirac model. Karplus curve, quadrupole broadening and decoupling, homotopic, enantiotopic and diastereotopic protons, virtual coupling, long range coupling. NOE and cross polarization.

3.3 2D NMR and COSY, HOMOCOSY and HETEROCOSY

3.5 Polarization transfer, selective population inversion, DEPT, sensitivity enhancement and MRI.

3.6 Problems on spectral interpretation with examples

Unit 4: Mass Spectrometry (9 Hrs)

4.1 Molecular ion: Ion production methods (EI). Soft ionization methods: SIMS, FAB, MALDI-TOF, Electrospray ionization, fragmentation patterns, alkyl halides, alcohols, phenols, aldehydes and ketones, esters amines, nitro compounds, acids, amides, nitrogen and ring rules, McLafferty rearrangement and its applications, HRMS, MS-MS, LC-MS, GC-MS.

4.2 Problems on spectral interpretation with examples.

Unit 5: Structural Elucidation Using Spectroscopic Techniques (9 Hrs)

5.1 Identification of structures of unknown organic compounds based on the data from UV-Vis, IR, ^{1}H NMR and ^{13}C NMR spectroscopy (HRMS data or Molar mass or molecular formula may be given).

5.2 Interpretation of the given UV-Vis, IR and NMR spectra.

5.3 Spectral analysis of the following reactions/functional transformations:

1. Pinacol-Pinacolone rearrangement
2. Benzoin condensation
3. Beckmann rearrangement
5. Benzil-benzilic acid rearrangement
7. Fries rearrangement

REFERENCES:

1. D.L. Pavia, G.M. Lampman, G.S. Kriz, *Introduction to Spectroscopy*, 3rd Edn., Brooks Cole, 2000.
2. A.U. Rahman, M.I. Choudhary, *Solving Problems with NMR Specroscopy, Academic Press*, 1996.
3. L. D. Field, S. Sternhell, J. R. Kalman, *Organic Structures from Spectra*, 4th Edn., John Wiley & sons, 2007.
4. C. N. Banwell, E.M. McCash, *Fundamentals of Molecular Spectroscopy*, 4th Edn., Tata McGraw Hill, 1994.
5. D. F. Taber, *Organic Spectroscopic Structure Determination: A Problem Based Learning Approach*, Oxford University Press, 2007.
6. H. Gunther, *NMR Spectroscopy*, 2nd Edn., Wiley, 1995.
7. R. M. Silverstein, G. C. Bassler, T. C. Morril, *Spectroscopic Identification of Organic Compounds*, 5th Edn., Wiley, 1991.
8. D. H. Williams, I. Fleming, *Spectroscopic Methods in Organic Chemistry*, 6th Edn. McGraw-Hill, 2008.
9. W. Kemp, *Organic Spectroscopy*, 2nd Edn., Macmillan, 1987.
10. F. Bernath, *Spectra of Atoms and Molecules*, 2nd Edn., Oxford University Press, 2005.
11. Online spectral databases including RIO-DB.

SEMESTER IV
ELECTIVE COURSES

24P4CHET13EL: ADVANCED INORGANIC CHEMISTRY

Credit: 4 **Contact Lecture Hours: 90**

After completing the course, the students will be able to:

	Course Outcome	*POs / PSOs*	*CL*	*KC*	*Class Sessions*
CO1	Apply the principles of group theory in co-ordination complexes.	PO 1 PSO 3	A	C	27
CO2	Identify the structure of an inorganic solid using IR, Raman, Mossbauer and EPR spectroscopic techniques.	PO 1 PSO 3	A	C	9
CO3	Explain the concepts of inorganic photochemistry.	PO 1 PSO 1	U	C	9
CO4	Describe the structure and properties of nanomaterials.	PO 1 PSO 1	R	F	18
CO5	Explain the chemistry of acids, bases, non-aqueous solvents and metal-organic frameworks.	PO 1 PSO 1	R	F	18
CO6	Explain the chemistry of fullerenes and metallo-supramolecular structures.	PO 1 PSO 1	R	F	9

Unit 1: Applications of Group Theory (27 Hrs)

1.1 Transformation properties of atomic orbitals, hybridization schemes for sigma and pi bonding with examples, symmetry adapted linear combination of atomic orbitals in tetrahedral, octahedral and sandwich complexes - ferrocene, formation of symmetry adapted group of ligand, MO diagrams.

1.2 Ligand field theory, splitting of *d* orbitals in different environments using group theoretical considerations, construction of energy level diagrams, correlation diagrams, method of descending symmetry, splitting terms for orbitals, energy levels, *d-d* transition-selection rules.

1.3 Determination of modes of vibrations in IR and Raman spectra using character tables in tetrahedral, octahedral and square planar complexes.

Unit 2: Inorganic Spectroscopic Methods (9 Hrs)

2.1 *Infrared and Raman Spectroscopy*: Structural elucidation of coordination compounds containing the following molecules/ions as ligands-NH_3, H_2O, CO, NO, $OH^–$, SO_4^{2-}, $CN^–$, $SCN^–$, NO_2^- and X^- (X=halogen).

2.2 *Electron Paramagnetic Resonance Spectroscopy*: EPR of d^1 and d^9 transition metal ions in cubic and tetragonal ligand fields, evaluation of g values and metal hyperfine coupling constants, electron-electron interactions.

2.3 *Mössbauer Spectroscopy*: Isomer shift, Quadrupole interaction, Magnetic hyperfine interaction. Applications of Mössbauer spectroscopy in the study of Fe complexes. Compound Identification- the interhalogen compound $I_2Br_2Cl_4$, iron in very high oxidation states – Fe (V) and Fe (VI) complexes.

Unit 3: Inorganic Photochemistry (9 Hrs)

3.1 Excited states in transition metal complexes: Intra-ligand excited states and metal centred excited states. Photochemical reactions: Substitution and redox reactions of Cr (III), Co (III), Rh (III) and Ru(II) complexes, manganese-based photosystems for the conversion of water into oxygen, applications-synthesis and catalysis, chemical actinometry and photochromism, dissociative photochemistry.

3.2 Metal complex sensitizers, electron relay, semiconductor supported metal oxide systems, water photolysis, nitrogen fixation and CO_2 reduction.

Unit 4: Nanomaterials (18 Hrs)

4.1 *Inorganic nanomaterials*: General introduction to nanomaterials, synthesis and applications of nanoparticles of gold, silver, rhodium, palladium and platinum, synthesis and applications of metal oxides of transition and non-transition elements-SiO_2, TiO_2, ZnO, Al_2O_3, iron oxides and mixed metal oxide nanomaterials, non-oxide inorganic nanomaterials, porous silicon nanomaterials- fabrication and chemical and biological sensing applications. Carbon nanotubes- preparation, properties and applications.

4.2 *Characterisation of Nanomaterials*: UV-visible, Raman, XRD, SEM, TEM and AFM techniques.

4.3. *Diversity in Nanosystems*: Self-assembled monolayers on gold-growth process and phase transition, quantum dots preparation, characterization and applications, nanoshells-types of systems, characterization and application

4.4. *Evolving Interfaces of Nanotechnology*: Nanocomposites- natural nanocomposites, polymer nanocomposites, metal and ceramic nanocomposites and clay nanocomposites. Nanobiotechnology, nano-biosensors, nanotechnology for manipulation of biomolecules- optical tweezers, dielectrophoresis, and biochips, nanocatalysts, nanomedicines- importance of nanomaterials in the pharmaceutical industry and future possibilities for medical nanotechnology, nanoparticles for medical imaging, nanoparticles for targeting cancer cells, nanoencapsulation for drug delivery to tumours.

Unit 5: Acids, Bases and Non-aqueous Solvents (9 Hrs)

5.1 Acid base concept in non-aqueous media-HSAB concept, solvent effects, linear free energy relationship-mechanism and methods of determination

5.2 Reactions in non-aqueous solvents. Ammonia - solutions of metals in liquid ammonia. Protonic solvents: anhydrous sulfuric acid, hydrogen halides. Aprotic solvents: non-polar solvents, non-ionizable polar solvents, polar solvents undergoing autoionization, liquid halogens, interhalogen compounds, oxy halides, dinitrogen tetroxide, sulphur dioxide.

Unit 6: Metal Organic Frame Works (9 Hrs)

6.1 Introduction, porous coordination polymers, frameworks with high surface area, Lewis acid frameworks, soft porous crystals, design of metal organic frameworks and design of functional metal organic frameworks by post-synthetic modification.

6.2 Applications of metal organic frameworks- separation and purification of gases by MOFs, hydrogen storage, MOFs in the pharmaceutical world.

Unit 7: Advanced Topics in Co-ordination Chemistry (9 Hrs)

7.1 Coordination Chemistry of Fullerenes. Fullerene metal complexes-Fullerides of alkali metals, Fullerenes as π-ligands, Metal fullerides, exohedral fullerenes, endohedral fullerenes. (*Only elementary study is expected*)

7.2 Metallo supra molecular chemistry and Molecular Architecture. Molecular recognition. Molecular Receptors and selective complexation for cation, anion and neutral molecules, Supramolecular Assistance in the Synthesis of Molecular and Supramolecular structures.

7.3 Diamondoid networks, inorganic crystal engineering using hydrogen bonds, organometallic crystal engineering, supramolecular self-assembly caused by ionic interactions- hydrocarbyls, amides and phosphides.

REFERENCES:

1. F. A. Cotton, *Chemical Applications of Group Theory*, Wiley-Interscience, 1990.
2. V. Ramakrishnan, M. S. Gopinathan, *Group Theory in Chemistry*, Vishal Pub., 1985.
3. A. S. Kunju, G. Krishnan, *Group Theory and its Applications in Chemistry*, PHI Learning, 2010
4. K. Nakamoto, *IR and Raman Spectra of Inorganic and Coordination Complexes, Part A Theory and Applications in Inorganic Chemistry*, 6^{th} Edn. John Wiley & sons, 1997.
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6. D. W. H. Rankin, N. W. Mitzel, C. A. Morrison, *Structural Methods in Molecular Inorganic Chemistry*, Wiley, 2013.
7. A. K. Bridson, *Inorganic Spectroscopic Methods*, Oxford University Press, 1998.
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9. D. M. Roundhill, *Photochemistry and Photophysics of Metal Complexes*, Plenum Press, 1994.
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20. J. E. Mark, H. R. Allock, R. West, *Inorganic Polymers*, 2^{nd} Edition, Oxford University Press, 2005.

SEMESTER IV
ELECTIVE COURSES

24P4CHET14EL: ADVANCED ORGANIC CHEMISTRY

Credit: 4 **Contact Lecture Hours: 90**

After completing the course, the students will be able to:

	Course Outcome	*POs / PSOs*	*CL*	*KC*	*Class Sessions*
CO1	Illustrate the principles of biosynthesis, biomimetic synthesis, green synthesis and stereoselective transformations.	PO 1 PSO 1	U	C	37
CO2	Explain the chemistry of advanced polymeric materials.	PO 1 PSO 4	A	C	13
CO3	Describe the structure and applications of natural products and biomolecules.	PO 1 PSO 1	U	C	14
CO4	Explain the mechanism of drug action and drug designing.	PO 1 PSO 1	U	C	16
CO5	Apply the methodology of research.	PO 1 PSO 1	U	C	10

Unit 1: Biosynthesis and Biomimetic Synthesis **(15 Hrs)**

1.1 Basic principles of the biosynthesis of terpenes, steroids, alkaloids, carbohydrates, and nucleic acids.

1.2 Biosynthesis of cholesterol.

1.3 Biogenesis of isoprenoids and alkaloids.

1.4 Structure of DNA and RNA. Replication of DNA - Flow of genetic information - Protein biosynthesis - transcription and translation - Genetic code - regulation of gene expression. Solid state synthesis of DNA.

Unit 2: Green Alternatives to Organic Synthesis **(12 Hrs)**

2.1 Principles of Green Chemistry: Basic concepts, atom economy - twelve principles of Green Chemistry - principles of green organic synthesis.

2.2 Green alternatives to Organic Synthesis: Coenzyme catalysed reactions -thyamine catalyzed benzoin condensation. Green alternatives of molecular rearrangements: Pinacol-pinacolone and Benzidine rearrangement. Electrophilic aromatic substitution reactions. Oxidation-reduction reactions. Clay catalysed synthesis. Condensation reactions. Green photochemical reactions.

2.3 Green Solvents: Ionic liquids, supercritical CO_2, fluorous chemistry.

2.4 General principles of microwave and ultrasound assisted organic synthesis.

Unit 3: Advances in Polymer Chemistry **(13 Hrs)**

3.1 Degree of polymerization, classification and stereochemistry of polymers. Ziegler-Natta catalyst. Glass transition temperature of polymers, factors affecting glass transition temperature.

3.2 *Conducting polymers* - temperature resistant and flame retardant polymers - polymers for medical applications.

3.3 *Dendrimers and dendritic polymers*: Terminology- classification of dendrimers. Methods of synthesis: convergent and divergent approaches. Dendrimers as nanocapsules. Applications of dendrimers.

3.4 *Hyper branched polymers*: definition, synthesis, applications.

Unit 4: Stereoselective Transformations **(10 Hrs)**

4.1 Assymetric induction- chiral auxiliaries and chiral pool.

4.2 Enantioselective catalytic hydrogenationdeveloped by Noyori and Knowels.

4.3 Assymetric aldol condensation pioneered by Evans.

4.4 Assymetric Diels- Alder reactions.

4.5 Assymetric epoxidation using Jacobsen's catalyst.

Unit 5: Chemistry of Natural Products and Biomolecules **(14 Hrs)**

5.1 Synthesis of camphor, atropine, papaverine, cyanin, quecertin, β-carotene, testosterone, PGE_2 and $PGF_{2\alpha}$, Vitamine C and Riboflavin.

5.2 Methods for primary structure determination of peptides, proteins.

5.3 Enzymes- classification, structure and mode of action.

Unit 6: Medicinal Chemistry and Drug Designing **(16 Hrs)**

6.1 Drug - Structure-activity relationships - a general idea.

6.2 Drug action - drug selectivity- receptor proteins- drug-receptor interaction - drug metabolism. Drug-receptor theory: occupancy theory, rate theory, induced fit theory, activation-aggregation theory. Mechanism of drug acting on DNA- intercalating agent (proflavin), alkylating agent (uracil mustard, *cis*-platin), chain cutting agents (bleomycin).

6.3 Central nervous system acting drugs (general idea), antidepressants, tranquilizers, sedatives and hypnotics.

6.4 A general idea of cardio-vascular drugs.

6.5 Introduction to Drug design- Concept of combinatorial and parallel synthesis. Computer assisted drug design. Illustration of drug development through a specific exampleof antibacterials- Pencillines.

Unit 7: Research Methodology of Chemistry (10 Hrs)

7.1 The search of knowledge - purpose of research - scientific methods - role of theory -

7.2 Characteristics of research. Types of research: Fundamental research, applied research, historical and experimental research.

7.3 *Statistical Calculations*: Presentation of data, mean, median, mode, errors in chemical analyses, linear regression and correlation. Method of least squares.

7.4 *Chemical Literature*: Primary, secondary and tertiary sources of literature. Classical and comprehensive reference. Literature databases: Science Direct, SciFinder. Chemical Abstract.

7.5 *Scientific Writing*: Research reports, thesis, journal articles, books. Types of publications: articles, communications, reviews.

7.6 Important scientific journals- important Chemistry journals. Impact factor

REFERENCES:

1. J. M. Lehn, *Supramolecular Chemistry: Concepts and Perspectives*, VCH, 1995.
2. F. Vogtle, *Supramolecular Chemistry: An Introduction*, Wiley, 1993.
3. W. Carruthers, I. Coldham, *Modern Methods of Organic Synthesis*, Cambridge University Press, 2004.
4. J. Clayden, N. Greeves, S. Warren, P. Wothers, *Organic Chemistry*, Oxford University Press, 2004.
5. R. O. C. Norman, J. M. Coxon, *Principles of Organic Synthesis*, Blackie Academic and Professional, 1993.
6. V. K. Ahluwalia, *Green Chemistry*, Ane Books, 2009.
7. J. M. Berg, J. L. Tymoczko, L. Stryer, *Biochemistry*, 6th Edn., W.H. Freeman, 2010.
8. A. L. Lehninger, D.L. Nelson, M.M. Cox, *Lehninger Principles of Biochemistry*, 5th Edn., W.H. Freeman, 2008.
9. V. K. Ahluwalia, M. Chopra, *Medicinal Chemistry*, Ane Books, 2008.
10. S. V. Bhat, B. A. Nagasampagi, M. Sivakumar, *Chemistry of Natural Products*, Narosa, 2005.
11. T. Pradeep, *Nano: the Essentials*, Tata McGraw Hill, 2007.
12. R. L. Dominoswki, *Research Methods*, Prentice Hall, 1981.
13. J. W. Best, J. V. Kahn, *Research in Education*, 10th Edn., Pearson/Allyn & Bacon, 2006.
14. H. F. Ebel, C. Bliefert, W. E. Russey, *The Art of Scientific Writing*, Wiley-VCH, 2004.
15. V. K. Ahluwalia, *Oxidation in Organic Synthesis*, CRC Press, 2012.
16. V. K. Ahluwalia, *Green Chemistry*, Narosa Publishing House, 2013
17. Jonathan W Steed & Jerry L Atwood, *Supramolecular Chemistry*, Wiley, 2nd Edition
18. Katsuhiko Ariga, Toyoki Kunitake, *Supramolecular Chemistry – Fundamentals and Applications*, Springer.

SEMESTER IV
ELECTIVE COURSES

24P4CHET15EL: ADVANCED PHYSICAL CHEMISTRY

Credit: 4 **Contact Lecture Hours: 90**

After completing the course, the students will be able to:

	Course Outcome	*POs / PSOs*	*CL*	*KC*	*Class Sessions*
CO1	Describe the physical principles of photochemistry.	PO 1 PSO 1	U	C	18
CO2	Explain the methods of fluorescence spectroscopy, electron diffraction and atomic spectroscopic techniques.	PO 1 PSO 1	U	C	18
CO3	Describe the principles of electrochemistry and applications of electromotive force.	PO 1 PSO 3	U	C	27
CO4	Apply various electro-analytical techniques in qualitative and quantitative analysis.	PO 1 PSO 1	A	C	18
CO5	Explain the principles of irreversible thermodynamics and bioenergetics.	PO 1 PSO 1	U	C	9

Unit 1: Photochemistry **(18 Hrs)**

1.1 Quantum yield, chemical actinometry, excimers and exciplexes, photosensitization, chemiluminescence, bioluminescence, thermoluminescence, pulse radiolysis, hydrated electrons, photostationary state, dimerization of anthracene, ozone layer in the atmosphere.

1.2 Principle of utilization of solar energy: solar cells, types of solar cells-amorphous silicon solar cell, cadmium telluride solar cell, copper indium gallium selenide solar cell.

1.3 Quenching of fluorescence and its kinetics, Stern-Volmer equation, concentration quenching, fluorescence and structure, delayed fluorescence, E-type and P-type, effect of temperature on emissions, photochemistry of environment, greenhouse effect, two photon absorption spectroscopy, lasers in photochemical kinetics.

Unit 2: Fluorescence Spectroscopy **(6 Hrs)**

2.1 Introduction, principle of fluorescence spectroscopy.

2.2 Instrumentation: light source, monochromator, optical filters, photomultiplier tube, polarizers.

2.3 Fluorophores – Intrinsic, Extrinsic, DNA probes, chemical sensing probes, green fluorescent proteins.

2.4 Fluorescence sensing, mechanism of sensing, sensing techniques based on collisional quenching, energy transfer and electron transfer, examples of pH sensors.

2.5 Novel fluorophores: lanthanides, long life time metal-ligand complexes.

Unit 3: Atomic Spectroscopic Techniques and Diffraction Methods (12 Hrs)

3.1 Atomic absorption spectroscopy (AAS): Principle of AAS. Instrumentation: light sources – hollow cathode lamp, electrodeless discharge lamp, different atomization techniques – flame, electrothermal, cold vapour atomization techniques, monochromator, detector. Interferences in AAS. Measurement of atomic absorption. Applications.

3.2 Atomic emission spectroscopy (AES): Principle and instrumentation. Origin of spectra, Excitation sources, Advantages and disadvantages of AES. Applications.

3.3 Flame emission spectroscopy (FES): Flames and flame temperature, Types of burners, spectra of metals in flame, instrumentation. Applications.

3.4 Electron diffraction of gases, Wierl's equation, Neutron diffraction method, Applications of neutron diffractions, Small angle neutron scattering.

Unit 4: Crystallography (12 Hrs)

4.1 Miller indices, point groups (derivation not expected), translational symmetry, glide planes and screw axes, space groups, simple cases like triclinic and monoclinic systems, interplanar spacing and method of determining lattice types, reciprocal lattices, methods of characterizing crystal structure, rotating crystal method, powder X-ray diffraction method, determination of structure of sodium chloride by powder method, comparison of the structures of NaCl and KCl, brief outline of single crystal X-ray diffraction and crystal growth techniques.

4.2 Structure factor: Atomic scattering factor, coordinate expression for structure factor, structure by Fourier synthesis.

Unit 5: Electrochemistry - II (18 Hrs)

4.2 Electrochemical cells, concentration cells and activity coefficient determination, liquid junction potential, evaluation of thermodynamic properties, the electrode double layer, electrode-electrolyte interface, different models of double layer, theory of multilayer capacity, electro capillary, Lippmann equation, membrane potential.

4.3 Fuel cells- Theory and working of fuel cells- methanol fuel cell, H_2-O_2 fuel cell and solid oxide fuel cells.

4.4 Corrosion and methods of prevention, Pourbaix diagram and Evans diagrams.

4.5 Overvoltage: hydrogen and oxygen overvoltage, theories of overvoltage, Tafel equation and its significance, Butler-Volmer equation for simple electron transfer reactions, transfer coefficient, exchange current density, rate constants.

Unit 5: Electroanalytical Techniques **(18 Hrs)**

5.1 *Voltametry*: Cyclic voltametry, anodic stripping voltametry.

5.2 *Polarography*: Decomposition potential, residual current, migration current, supporting electrolyte, diffusion current, polarogram, half wave potential, limiting current density, polarograph, explanation of polarographic waves.

5.3 The dropping mercury electrode, advantages and limitations of DME, quantitative analysis - pilot ion procedure, standard addition methods, qualitative analysis determination of half wave potential of an ion, advantages of polarography.

5.4 *Amperometric titrations*: General principles of amperometry, instrumentation, application of amperometry in the qualitative analysis of anions and cations in solution, merits and demerits of amperometric titrations.

5.5 *Coulometry*: Coulometer-Hydrogen Oxygen coulometers, silver coulometer, coulometric analysis with constant current, coulometric titrations, application of coulometric titrations-neutralization titrations, complex formation titrations, redox titrations, advantages of coulometry.

Unit 6: Advanced Thermodynamics **(6 Hrs)**

6.1 Thermodynamics of irreversible processes, general theory of non-equilibrium processes, entropy production, the phenomenological relations, the principle of microscopic reversibility, Onsager reciprocal relations, thermal osmosis and thermoelectric phenomena.

6.2 Bioenergetics, coupled reactions, ATP and its role in bioenergetics, high energy bond, free energy and entropy change in ATP hydrolysis, thermodynamic aspects of metabolism and respiration, glycolysis, biological redox reactions.

REFERENCES:

1. K. K. Rohatgi-Mukherjee, *Fundamentals of Photochemistry*, 2nd Edn. New Age International, 1986.
2. G. Aruldhas, *Molecular structure and Spectroscopy*, PHI Learning, 2007.
3. B. Valeur, *Molecular Fluorescence: Principles and Applications*, Wiley-VCH 2002.
4. J. R. Lakowicz, *Principles of Fluorescence Spectroscopy*, 3rd Edn., Springer, 2006.
5. D. L. Andrews, A. A. Demidov, *Resonance Energy Transfer*, Wiley, 1999.
6. R. J. Silbey, R. A. Alberty, M. G. Bawendi, *Physical Chemistry*, 4th Edn., Wiley, 2005.
7. G. M. Barrow, *Physical Chemistry*, 5th Edn., Tata McGraw Hill, 2007.
8. K. J. Laidler, J. H. Meiser, B.C. Sanctuary, *Physical Chemistry*, 4th Edn., Houghton Mifflin, 2003.
9. P. W. Atkins, *Physical Chemistry*, ELBS, 1994.
10. G. W. Castellan, *Physical Chemistry*, Addison-Wesley, 1983.
11. S. Glasstone, *Introduction to Electrochemistry*, Biblio Bazar, 2011.
12. D. R. Crow, *Principles and Applications of Electrochemistry*, 4th Edn. S.Thornes, 1994.
13. B. K. Sharma, *Electrochemistry*, Krisna Prakashan, 1985.
14. John O'M Bockris and Amulya K.N. Reddy, *Modern Electrochemistry* Vol I & II Springer International Edn.2006.
15. H. Kaur, *Spectroscopy*, 6th Edn., Pragati Prakashan, 2011.
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17. H. H. Willard, J.A .Dean, L.L. Merritt, *Instrumental Methods of Analysis*, Van Nostrand, 1965.
18. D. A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, *Fundamentals of Analytical Chemistry*, 8th Edn., Saunders College Pub., 2007.
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20. J. Rajaram, J. C. Kuriakose, *Thermodynamics*, S Chand and Co., 1999
21. R. K. Murray, D. K. Granner, P. A. Mayes, V. W. Rodwell, *Harper's Biochemistry*, Tata McGraw Hill, 1999.
22. I. Tinoco, K. Sauer, J.C. Wang, J.D. Puglisi, *Physical Chemistry: Principles and Applications in Biological Science*, Prentice Hall, 2002

SEMESTERS III & IV

24P4CHEP04: INORGANIC CHEMISTRY PRACTICAL - II

Credit: 3 **Contact Lab Hours: 54 + 54 =108**

After completing the course, the students will be able to:

	Course Outcome	*POs / PSOs*	*CL*	*KC*	*Class Sessions*
CO1	Estimate binary mixtures of metallic ions in solution.	PO 1 PSO 5	A	P	54
CO2	Synthesize and characterize nanomaterials.	PO 1 PSO 5	A	P	54

PART I

Estimation of simple binary mixtures (like Cu-Ni, Cu-Zn, Fe-Cr, Fe-Cu, Fe-Ni, Pb-Ca) of metallic ions in solution by volumetric and gravimetric methods.

PART II

Introduction to material science and Nanotechnology

- Green synthesis of nanoAg/nanoAu-Assigning SPR band using UV-Vis Spectroscopy
- Synthesis of nano silica/nano titania- FTIR characterization
- Synthesis of nano Zinc Oxide- FTIR characterization
- Synthesis of nanocellulose- FTIR characterization
- Synthesis of the conducting polymer-poly aniline- FTIR characterization
- Synthesis of PbS/CdS/CdSe/ZnS quantum dot-UV- Vis spectral characterization

References

01. A.I. Vogel, *A Text Book of Quantitative Inorganic Analysis*, Longman, 1966.
02. I.M. Koltoff, E.B. Sandell, *Text Book of Quantitative Inorganic Analysis*, 3rd Edn. Mc Millian, 1968.
03. G. Pass, H. Sutcliffe, *Practical Inorganic Chemistry*, Chapman & Hall, 1974.
04. N.H. Furman, *Standard Methods of Chemical Analysis*: Volume 1, Van Nostrand, 1966.
05. F.J. Welcher, *Standard Methods of Chemical Analysis*: Vol. 2, R.E. Kreiger Pub., 2006
06. T. Pradeep, *Nano: the Essentials*, Tata Mc Graw Hill, 2007.
07. C.N.R. Rao, A. Govindaraj, *Nanotubes and Nanowires*, Royal Society of Chemistry, 2011.

SEMESTERS III & IV

24P4CHEP05: ORGANIC CHEMISTRY PRACTICAL - II

Credit: 3 **Contact Lab Hours: 54 + 54 =108**

After completing the course, the students will be able to:

	Course Outcome	***POs / PSOs***	***CL***	***KC***	***Class Sessions***
CO1	Carry out multi-step organic synthesis	PO 1 PSO 5	A	P	27
CO2	Purify the synthesized organic compounds	PO 1 PSO 5	A	P	18
CO3	Synthesize organic compounds using green alternative methods.	PO 1 PSO 5	A	P	36
CO4	Record and interpret IR spectrum of a compound	PO 1 PSO 5	A	P	9
CO5	Explain the method of molecular docking studies.	PO 1 PSO 5	A	P	18

PART I

Preparation and purification of organic compounds involving Two step Synthetic Sequences by Chemical Methods (Reactions involving nitration, Bromination, deamination, hydrolysis, rearrangement etc.)

PART II

Preparation Involving Multistep Synthetic Sequences by the Green Alternatives of Chemical Methods including Enzyme/coenzyme catalysed reactions

PART III

Microwave assisted Organic Synthesis - oxidation, hydrolysis, condensation, substitution *etc*.

PART IV

Record the IR spectrum of the compounds synthesised in part I-III.

Generate and interpret the 1H and ^{13}C NMR spectra of selected organic molecules using software.

PART V

Study of enzyme- drug interaction by molecular docking (*Minimum three models*)

REFERENCES:

1 A.I.Vogel, *A Textbook of Practical Organic Chemistry*, Longman, 1989.

2 A.I.Vogel, *Elementary Practical Organic Chemistry*, Longman, 1957.

3 F.G. Mann, B.C Saunders, *Practical Organic Chemistry*, 2009.

4 J.R. Johnson, J.F.Wilcox, *Laboratory Experiments in Organic Chemistry*, Macmillan, 1979.

5 V.K. Ahluwalia, *Green Chemistry : Environmentally Benign Reactions*, Ane Books, New Delhi, 2009.

6 Monograph on Green Chemistry Laboratory Experiments, Green Chemistry Task Force Committee, DST, 2009.

7. Patric, G. L., *An Introduction to Medicinal Chemistry*. 5thEdn.; Oxford University,2013.

SEMESTERS III & IV

24P4CHEP06 : PHYSICAL CHEMISTRY PRACTICAL - II

Credit: 3 **Contact Lab Hours: 72 + 72 = 144**

After completing the course, the students will be able to:

	Course Outcome	***POs / PSOs***	***CL***	***KC***	***Class Sessions***
CO1	Carry out experiments related to chemical kinetics, viscometry, Polarimetry, Refractometry, Conductometry and Potentiometry.	PO 1 PSO 5	A	P	144

I Chemical Kinetics

1. Determination of the rate constant of the hydrolysis of ester by sodium hydroxide/HCl
2. Determination of Arrhenius parameters.
3. Kinetics of reaction between $K_2S_2O_8$ and KI
4. Influence of ionic strength on the rate constant of the reaction between $K_2S_2O_8$ and KI
5. Iodination of acetone in acid medium.

II Polarimetry

1. Kinetics of the inversion of sucrose in presence of HCl.
2. Determination of the concentration of a sugar solution.
3. Determination of the concentration of HCl.
4. Determination of the relative strength of acids.

III Refractometry

1. Determination of molar refractions of pure liquids.
2. Determination of concentration of solutions (KCl-water, glycerol-water).
3. Determination of molar refraction of solids.
4. Study of complex formation between potassium iodide and mercuric iodide system.

IV Conductivity measurements

1. Verification of Onsager equation.
2. Determination of the degree of ionization of weak electrolytes.

3. Determination of pKa values of organic acids.
4. Determination of solubility of sparingly soluble salts.
5. Titration of a strong acid/Weak acid against a strong base.
6. Titration of a dibasic acid against a strong base.
7. Conductometric determination of the rate constant for the alkaline hydrolysis of methyl acetate.

V Potentiometry

1. Determination of single electrode potentials (Cu and Zn).
2. Application of Henderson equation.
3. Titration of a mixture of acids against a strong base.
4. Redox Titrations and determination of formal redox potential.

VI Cyclic Voltammetry

1. Determination of diffusion coefficient.
2. Study of scan rate dependent behavior.

REFERENCES:

1. J.B. Yadav, *Advanced Practical Physical Chemistry*, Goel Publishing House, 2001.
2. G.W. Garland, J.W. Nibler, D.P. Shoemaker, *Experiments in Physical Chemistry*, 8^{th} Edn. McGraw Hill, 2009.
3. B. Viswanathan, *Practical Physical chemistry*, Viva Pub., 2005
4. Saroj Kumar and Naba Kumar, *Physical Chemistry Practical*, New Central Book Agency, 2012
5. Practical Physical Chemistry Paperback, 1974 by A.M. James, F.E. Prichard.

24P4CHECV - Comprehensive Viva Voce

There will be a comprehensive viva at the end of the programme, which covers questions from all courses in the programme as per the syllabus.

The viva board consists of three external examiners preferably same as the practical examiners for the respective subject and one internal examiner (Class teacher).

24P4CHEPJ - Project

- Each student should submit a project report for evaluation. Project work shall be completed by working outside the regular teaching hours.
- A minimum of 3 months period shall be given to each student for the project and this may be after the end semester examination of semester 4.
- Project work shall be carried out under the supervision of a teacher in the concerned department or an external supervisor.
- Students can do their project in the department or any other reputed research institution in and outside the state.
- There should be an internal assessment and external assessment for the project work in the ratio 1:3.
- After completing the project the report should be submitted to the department for internal and external evaluation.
- The external evaluation of the project work consists of valuation of the dissertation (project report) followed by presentation of the work and viva voce.
- The external evaluation will be done by the project viva board, which consists of three examiners.
- The grade and credit with grade awarded for the program project should be entered in the grade card issued by the college.