

**M.Sc. CHEMISTRY**  
**CHOICE BASED CREDIT SYSTEM**  
**(CBCS)**

Syllabus  
2021-2022



**DEPARTMENT OF CHEMISTRY**  
FACULTY OF ARTS, SCIENCE AND HUMANITIES

**KARPAGAM ACADEMY OF HIGHER EDUCATION**

*(Deemed to be University)*

*(Established Under Section 3 of UGC Act, 1956)*

Pollachi Main Road, Eachanari (Post), Coimbatore- 641 021,  
Tamil Nadu, India

Phone: 0422 – 2980011 – 15 Fax No: 0422 – 2980022-23

Email: [info@karpagam.com](mailto:info@karpagam.com) Web: [www.kahedu.edu.in](http://www.kahedu.edu.in)

# **KARPAGAM ACADEMY OF HIGHER EDUCATION**

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Coimbatore - 641 021, INDIA

## **FACULTY OF ARTS, SCIENCE AND HUMANITIES POST-GRADUATE PROGRAMMES (M.Sc., M.Com.)**

### **REGULAR MODE CHOICE BASED CREDIT SYSTEM (CBCS)**

#### **REGULATIONS - 2021**

The following Regulations are effective from the academic year 2021-2022 and are applicable to the candidates admitted in Post Graduate (PG) Degree programmes in the Faculty of Arts, Science, and Humanities, Karpagam Academy of Higher Education (KAHE).

#### **1 PROGRAMMES OFFERED,**

#### **MODE OF STUDY AND ADMISSION REQUIREMENTS**

#### **1.1 P.G. PROGRAMMES OFFERED**

The various P.G. Programmes offered by the KAHE are listed in the table below.

<b>S. No.</b>	<b>Programme Offered</b>
1	M.Sc. Biochemistry
2	M.Sc. Microbiology
3	M.Sc. Biotechnology
4	M.Sc. Physics
5	M.Sc. Chemistry
6	M.Sc. Mathematics
7	M.Sc. Computer Science
8	M.Sc. Applied Astrology
9	M.Com.

## 1.2 MODE OF STUDY

### Full-Time

All programmes are offered under Full-Time Regular mode. Candidates admitted under 'Full-Time' should be present in the KAHE during the complete working hours for curricular, co-curricular and extra-curricular activities assigned to them.

### 1.3 ADMSSION REQUIREMENTS (ELIGIBILITY)

Candidates for admission to the first semester Master's Degree Programme shall be required to have passed an appropriate Degree Examination of this Karpagam Academy of Higher Education or any other University accepted by the KAHE as equivalent thereto. Admission shall be offered only to the candidates who possess the qualification prescribed against each course as given in the table below.

### QUALIFICATIONS FOR ADMISSION

S. No.	Name of the Programme Offered	Eligibility
1	M.Sc. Biochemistry	B.Sc. Degree with Biology / Biochemistry / Chemistry / Biotechnology / B.F.Sc. / Polymer Chemistry / Microbiology/ Zoology / Botany / Plant Science / Plant Biotechnology / Animal Science / Animal Biotechnology / B.Pharm / Industrial Chemistry / Applied Microbiology / Medical Microbiology / Human Genetics / Medical Genetics / Molecular Biology / Genetics Technology / Environmental Science / Environment Biotechnology / Genetics Engineering / Bioinformatics / Plant Biology & Biotechnology / Animal Cell & Biotechnology / Agriculture / Medical Lab Technology / Nutrition & Dietetics
2	M.Sc. Microbiology	B.Sc. Microbiology / Applied Microbiology / Industrial Microbiology / Medical Microbiology / Botany / Zoology / Biology / Biotechnology / Molecular Biology / Genetic Engineering / Biochemistry / Agriculture / Forestry / Medical Lab Technology / Life Sciences
3	M.Sc. Biotechnology	B.Sc. Degree with Biology / Biochemistry / B.Sc Biology with Chemistry Ancillary / B.F.Sc. / Microbiology / Zoology / Botany / Plant Science /Plant Biotechnology / Animal Science /Animal Biotechnology / B.Pharm / Applied Microbiology / Medical Microbiology / Human Genetics / Medical

		Genetics / Molecular Biology / Genetics / Environmental Science / Environment Biotechnology / Genetics Engineering / Bioinformatics / Plant Biology & Biotechnology / Animal Cell & Biotechnology / Agriculture / B.Tech ( Biotech)
4	M.Sc. Physics	B.Sc. Physics, B.Sc. Physics (CA) / B.Sc. Applied science
5	M.Sc. Chemistry	B. Sc. Chemistry, Industrial Chemistry, Polymer Chemistry
6	M.Sc. Mathematics	B.Sc. Mathematics / B.Sc. Mathematics with Computer Applications
7	M.Sc. Computer Science	B.Sc. Computer Science / Computer Technology / Information Technology / Electronics / Software Systems / BCA/ B.Sc. Applied Sciences
8	M.Sc. Applied Astrology	B.Sc. Allied Astrology or Equivalent degree
9	M.Com	B.Com./BCom.(CA)/B.Com(PA)/B.Com(Finance& Insurance)/ B.Com.(e-Commerce)/ B.Com.(IT) /B.B.M. /B.B.M.(CA) /B.B.A./B.B.A (CA) / B.Com (CS), B.A. Co-Operation / Bachelor's Degree in Bank Management/ B.A. Economics / B. Com Financial Analytics/ B. Com International Accounting and Finance

## 2 DURATION OF THE PROGRAMMES

2.1 The minimum and maximum period for completion of the P.G. Programmes are given below:

Programme	Min. No. of Semesters	Max. No. of Semesters
M.Sc., M.Com	4	8

2.2 Each semester normally consists of 90 working days or 450 Instructional hours for full-time mode of study. Examination shall be conducted at the end of every semester for the respective courses.

## 3. CHOICE BASED CREDIT SYSTEM

3.1 All programmes are offered under Choice Based Credit System with a total credit ranges from 87 to 93 for the PG programmes.

### **3.2 Credits**

Credits means the weightage given to each course of study by the experts of the Board of Studies concerned. A total of 87 to 93 credits are prescribed for the PG programme (two years)

### **4. STRUCTURE OF THE PROGRAMME**

Every Programme will have a curriculum and syllabus consisting of core courses, elective courses, open elective and project work.

#### **a. Core course**

Core course consists of theory and practical and the examinations shall be conducted at the end of each semester.

#### **b. Elective course**

Elective courses are to be chosen with the approval of the Head of Department concerned from the list of elective courses mentioned in the curriculum.

#### **c. Project Work**

The candidates shall undertake the project work in the Fourth Semester either in the Department concerned or in Industries, Institute or any other Organizations and the project report has to be submitted at the end of the fourth semester.

In case the candidate undertakes the project work outside the Department, the teacher concerned within the Department shall be the Main guide and the teacher/scientist under whom the work is carried out will be the Co-guide. The candidate shall bring the attendance certificate from the place of project work carried out.

#### **d. Value Added Courses**

Courses of varying durations but not less than 30 hours which are optional and offered outside the curriculum that add value and help the students in for getting placement. Students of all programmes are eligible to enroll for the Value Added Courses. The student shall choose one Value Added Course per semester from the list of Value Added Courses available in KAHE. The examinations shall be conducted at the end of the Value Added Course at the Department level and the student has to secure a minimum of 50% of marks to get a pass. The certificate for the Value Added Course for the passed out students shall be issued duly signed by the HOD and Dean of the Faculty concerned.

#### **e. Internship**

The student shall undergo 15 days internship in the end of second semester.

#### **Online Course**

Student shall study at least one online course from SWAYAM / NPTEL / MOOC in any one of the first three semesters for which examination shall be conducted at the end of the course by the respective external agencies if any. The student can register to the courses which are approved by the Department. The student shall produce a Pass Certificate from the respective agencies before the end of the third semester. The

credit(s) earned by the students will be considered as additional credit(s) over and above the credits minimum required to earn a particular Degree.

### **5. MEDIUM OF INSTRUCTION**

The medium of instruction for all courses, examinations, seminar presentations and project/thesis/dissertation reports should be in English.

### **6. MAXIMUM MARKS**

The maximum marks assigned to different courses shall be as follows:

- (i) Each of the theory and practical courses shall carry maximum of 100 marks. Out of which 40 marks are for Continuous Internal Assessment (CIA) and 60 marks for End Semester Examinations (ESE).

(ii) **Maximum marks for Project work**

<b>S. No</b>	<b>Programme</b>	<b>Maximum marks</b>	<b>CIA</b>	<b>ESE</b>
1	M.Sc., M.Com.	200	80	120

### **7. REQUIREMENTS TO APPEAR FOR THE END SEMESTER EXAMINATION**

a. Ideally every student is expected to attend all classes and secure 100% attendance. However, in order to allow for certain unavoidable circumstances, the student is expected to attend at least 75% of the classes and the conduct of the candidate is satisfactory during the course.

b. A candidate who has secured attendance between 65% and 74% (both included), due to medical reasons (Hospitalization / Accident / Specific Illness) or due to participation in University / District / State / National / International level sports or due to participation in Seminar / Conference / Workshop / Training Programme / Voluntary Service / Extension activities or similar programmes with prior permission from the Registrar shall be given exemption from prescribed minimum attendance requirements and shall be permitted to appear for the examination on the recommendation of the Head of Department concerned and Dean to condone the shortage of attendance. The Head of Department has to verify and certify the genuineness of the case before recommending to the Dean. However, the candidate has to pay the prescribed condonation fee to the KAHE.

c. However, a candidate who has secured attendance less than 64% in the current semester due to any reason shall not be permitted to appear for the current semester examinations. But he/she will be permitted to appear for his/her supplementary examinations, if any and he/she has to re do the same semester with the approval of the “Students’ Affairs Committee” and Registrar.

## **8. a. FACULTY MENTOR**

To help students in planning their courses of study and for general advice on the academic programme, the HoD shall allot a certain number of students to a faculty who will function as mentor throughout their period of study. Faculty mentors shall advise the students and monitor their behavior and academic performance. Problems if any shall be counseled by them periodically. The Faculty mentor is also responsible to inform the parents of their wards progress. Faculty mentor shall display the cumulative attendance particulars of his / her ward students' periodically (once in 2 weeks) on the Notice Board to enable the students to know their attendance status and satisfy the **clause 7** of this regulation.

## **b. ONLINE COURSE COORDINATOR**

To help students in planning their online courses and for general advice on online courses, the HOD shall nominate a coordinator for the online courses. The Online course coordinator shall identify the courses which the students can select for their programme from the available online courses offered by the different agencies periodically and inform the same to the students. Further, the coordinators shall advice the students regarding the online courses and monitor their course.

## **9. CLASS COMMITTEE**

Every class shall have a Class Committee consisting of teachers of the class concerned, student representatives (Minimum two boys and 2 girls of various capabilities and Maximum of 6 students) and the concerned HoD / senior faculty as a Chairperson. The objective of the class committee Meeting is all about the teaching – learning process. Class Committee shall be convened at least once in a month. The functions of the Class Committee shall include

- Analyzing and Solving problems experienced by students in the class room and in the laboratories.
- Analyzing the performance of the students of the class after each test and finding the ways and means to improve the performance.
- The Class Committee of a particular class of any department is normally constituted by the HoD / Chairperson of the Class Committee. However, if the students of different departments are mixed in a class, the class committee shall be constituted by the respective faculty Dean.
- The Class Committee shall be constituted during the first week of each semester.
- The HoD / Chairperson of the class committee are authorized to convene the meeting of the class committee.

- The respective faculty Dean has the right to participate in any class committee meeting.
- The Chairperson is required to prepare the minutes of every meeting, and submit the same to Dean within two days after having convened the meeting. Serious issues if any shall be brought to the notice of the Registrar by the HoD / Chairperson immediately.

## 10. COURSE COMMITTEE FOR COMMON COURSES

Each common theory course offered to more than one discipline or group shall have a “Course Committee” comprising all the teachers handling the common course with one of them nominated as course coordinator. The nomination of the course coordinator shall be made by the Dean depending upon whether all the teachers handling the common course belong to a single department or to various other departments. The ‘Course Committee’ shall meet in order to arrive at a common scheme of evaluation for the tests to ensure a uniform evaluation of the tests. If feasible, the course committee shall prepare a common question paper for the Internal Assessment test(s).

## 11. PROCEDURE FOR AWARDING MARKS FOR INTERNAL ASSESSMENT

11.1 Every Faculty is required to maintain an **Attendance and Assessment Record (Log book)** which consists of attendance of students marked for each lecture / practical / project work class, the test marks and the record of class work (topic covered), separately for each course. This should be submitted to the HoD once in a fortnight for checking the syllabus coverage and records of test marks and attendance. The HoD shall sign with date after due verification. The same shall be submitted to Dean once in a month. After the completion of the semester the HoD should keep this record in safe custody for five years. Because records of attendance and assessment shall be submitted for inspection as and when required by the KAHE / any other approved body.

11.2 **Continuous Internal Assessment (CIA)**: The performance of students in each course will be continuously assessed by the respective faculty as per the guidelines given below:

### Theory Courses

S. No.	Category	Maximum Marks
1	Attendance	5
2	Test – I (first 2 ½ units)	10
3	Test – II (last 2 ½ units)	10
4	Journal Paper Analysis & Presentation*	15
<b>Continuous Internal Assessment : Total</b>		<b>40</b>



\*Evaluated by two faculty members of the department concerned. Distribution up of marks for one Journal paper analysis: Subject matter 5 marks, Communication/PPT Presentation 4 marks, Visual aid 2 marks and Question and Discussion 4 marks

### Practical Courses

S. No.	Category	Maximum Marks
1	Attendance	5
2	Observation work	5
3	Record work	5
4	Model practical examination	15
5	<i>Viva – voce</i> [Comprehensive]*	10
<b>Continuous Internal Assessment: Total</b>		<b>40</b>

\* *Viva - voce* conducted during model practical examination.

Every practical Exercise / Experiment shall be evaluated based on the conduct of Exercise/ Experiment and records maintained.

### 11.3 Pattern of Test Question Paper

Instruction	Remarks
Maximum Marks	50 marks
Duration	2 Hours
Part – A	Objective type (20x1=20)
Part - B	Short Answer Type (3 x 2 = 6)
Part - C	3 Eight marks questions ‘either – or’ choice (3 x 8 = 24 Marks)

11.4

### Attendance

#### Marks Distribution for Attendance

S. No.	Attendance (%)	Maximum Marks
1	91 and above	5.0
2	81 - 90	4.0

3	76 - 80	3.0
4	Less than 75	0

## 12. ESE EXAMINATIONS

**12.1 End Semester Examination (ESE):** ESE will be held at the end of each semester for each course. The question paper is for a maximum of 60 marks.

Pattern of ESE Question Paper

<b>Instruction</b>	<b>Remarks</b>
Maximum Marks	60 marks for ESE
Duration	3 hours (½ Hr for Part – A Online & 2 ½ Hours for Part – B and C)
Part – A	20 Questions of 1 mark each (20 x 1 = 20 Marks) Question No. 1 to 20 Online Multiple Choice Questions
Part- B	5 Questions of six marks each (5 x 6 = 30 Marks.) Question No. 21 to 25 will be ‘either-or’ type, covering all five units of the syllabus; i.e., Question No. 21: Unit - I, either 21 (a) or 21 (b), Question No. 22: Unit - II, either 22 (a) or 22 (b), Question No. 23: Unit - III, either 23 (a) or 23 (b), Question No. 24: Unit - IV, either 24 (a) or 24 (b), Question No. 25: Unit - V, either 25 (a) or 25 (b)
Part - C	Question No.26. One Ten marks Question (1 x 10 = 10 Marks)

**12.2 Practical:** There shall be combined valuation. The pattern of distribution of marks shall be as given below.

Experiments	: 40 Marks
Record	: 10 Marks
Viva-voce	: 10 Marks
<b>Total</b>	<b>: 60 Marks</b>

### **Record Notebooks for Practical Examination**

Candidate taking the Practical Examination should submit Bonafide Record Notebook prescribed for the Practical Examination, failing which the candidate will not be permitted to take the Practical Examination.

In case of failures in Practical Examination, the marks awarded for the Record at the time of first appearance of the Practical Examination shall remain the same at the subsequent appearance also by the candidate.

### 12.3. Evaluation of Project Work

12.3.1 The project shall carry a maximum marks as per clause 6 (ii). ESE will be a combined evaluation of Internal and External Examiners.

12.3.2 The project report is prepared according to the approved guidelines and duly signed by the supervisor(s) shall be submitted to HoD.

Guidelines to prepare the project report

- a. Cover page
- b. Bonafide certificate
- c. Declaration
- d. Acknowledgement
- e. Table of contents
- f. Chapters

Introduction

Aim and Objectives

Materials and Methods (Methodology)

Results (Analysis of Data) and Discussion (Interpretation)

Summary

References

12.3.3 The evaluation of the project will be based on the project report submitted and *Viva-Voce* Examination by a team consisting of the supervisor, who will be the Internal Examiner and an External Examiner who shall be appointed by the COE. In case the supervisor is not available, the HoD shall act as an Internal Examiner.

12.3.4 If a candidate fails to submit the project report on or before the specified date given by Examination Section, the candidate is deemed to have failed in the project work and shall re-enroll for the same in a subsequent semester.

If a candidate fails in the *viva-voce* examinations he/she has to resubmit the project report within 30 days from the date of declaration of the results. For this purpose the same Internal and External examiner shall evaluate the resubmitted report.

12.3.5 Copy of the approved project report after the successful completion of *viva voce* examinations shall be kept in the KAHE library.

### **13. PASSING REQUIREMENTS**

- 13.1 Passing minimum: There is a passing minimum 20 marks out of 40 marks for CIA and the passing minimum is 30 marks out of 60 marks in ESE. The overall passing in each course is 50 out of 100 marks (Sum of the marks in CIA and ESE examination).
- 13.2 If a candidate fails to secure a pass in a particular course (either CIA or ESE or Both) as per clause 13.1, it is mandatory that the candidate has to register and reappear for the examination in that course during the subsequent semester when examination is conducted for the same till he/she secures a pass both in CIA and ESE (vide Clause 2.1).
- 13.3 Candidate failed in CIA will be permitted to improve CIA marks in the subsequent semesters by writing tests and by re-submitting assignments.
- 13.4 CIA marks (if it is pass) obtained by the candidate in the first appearance shall be retained by the Office of the Controller of Examinations and considered valid for all subsequent attempts till the candidate secures a pass in ESE.
- 13.5 A candidate who is absent in ESE in a Course / Practical / Project work after having enrolled for the same shall be considered to have **failed** in that examination.

### **14. IMPROVEMENT OF MARKS IN THE COURSE ALREADY PASSED**

Candidates desirous to improve the marks secured in a passed course in their first attempt shall reappear once (**only in ESE**) in the subsequent semester. **The improved marks shall be considered for classification but not for ranking.** If there is no improvement there shall be no change in the marks awarded earlier.

## 15. AWARD OF LETTER GRADES

All assessments of a course will be done on absolute marks basis. However, for the purpose of reporting the performance of a candidate, letter grades, each carrying certain number of points, will be awarded as per the range of total marks (out of 100) obtained by the candidate in each course as detailed below:

Letter grade	Marks Range	Grade Point	Description
O	91 - 100	10	OUTSTANDING
A+	81- 90	9	EXCELLENT
A	71-80	8	VERY GOOD
B+	66- 70	7	GOOD
B	61 – 65	6	ABOVE AVERAGE
C	55 - 60	5	AVERAGE
D	50 - 54	4	PASS
RA	<50	-	REAPPEARANCE
AAA	-	-	ABSENT

## 16. GRADE SHEET

After the declaration of the results, Grade Sheets will be issued to each student which will contain the following details:

- i. The list of courses enrolled during the semester and the corresponding grade scored.
- ii. The Grade Point Average (**GPA**) for the semester and
- iii. The Cumulative Grade Point Average (**CGPA**) of all courses enrolled from first semester onwards.

GPA of a Semester and CGPA of a programme will be calculated as follows.

$$\text{GPA of a Semester} = \frac{\text{Sum of the product of the GP by the corresponding credits of the courses offered in that Semester}}{\text{Sum of the credits of the courses of that Semester}}$$

$$\frac{\sum_i C_i G P_i}{\sum_i C_i}$$

i.e. **GPA** of a Semester =

Sum of the product of the GPs by the corresponding credits of the courses offered for the entire programme

**CGPA** of the entire programme =  $\frac{\text{Sum of the product of the GPs by the corresponding credits of the courses offered for the entire programme}}{\text{Sum of the credits of the courses of the entire programme}}$

$$\text{i.e. CGPA of the entire programme} = \frac{\sum_n \sum_i C_{ni} GP_{ni}}{\sum_n \sum_i C_{ni}}$$

where,

$C_i$  is the credit fixed for the course 'i' in any semester

$GP_i$  is the grade point obtained for the course 'i' in any semester

'n' refers to the Semester in which such courses are credited

**Note:** RA grade will be excluded for calculating **GPA** and **CGPA**.

## 17. REVALUATION

Candidate can apply for revaluation and retotalling of his / her semester examination answer script (**theory courses only**), within 2 weeks from the date of declaration of results, on payment of a prescribed fee. For the same, the prescribed application has to be sent to the Controller of Examinations through the HoD. **A candidate can apply for revaluation of answer scripts not exceeding 5 courses at a time.** The Controller of Examinations will arrange for the revaluation and results will be intimated to the candidate through the HODs concerned. Revaluation is not permitted for supplementary theory courses.

## 18. TRANSPARENCY AND GRIEVANCE COMMITTEE

Revaluation and Re-totalling is allowed on representation (clause 17). Student may get the Xerox copy of the answer script on payment of prescribed fee, if he / she wish. The student may represent the grievance, if any, to the Grievance Committee, which consists of Dean of the Faculty, (if Dean is HoD, the Dean of another Faculty nominated by the KAHE), the HoD of Department concerned, the faculty of the course and Dean from other discipline nominated by the KAHE and the CoE. If the Committee feels that the grievance is genuine, the script may be sent for external

valuation; the marks awarded by the External examiner will be final. The student has to pay the prescribed fee for the same.

## **19. ELIGIBILITY FOR THE AWARD OF THE DEGREE**

**A student shall be declared to be eligible for the conferment of the Degree if he / she has**

- Successfully completed all the components in clause 3 and gained the required number of total credits as specified in the curriculum corresponding to his / her Programme within the stipulated period.
- Not any disciplinary action pending against him / her.
- The award of the degree must be approved by the Board of Management.

## **20. CLASSIFICATION OF THE DEGREE AWARDED**

20.1 Candidate who qualifies for the award of the Degree (vide clause 13) having passed the examination in all the courses in his / her first appearance, within the specified minimum number of semesters and securing a **CGPA not less than 8.0** shall be declared to have passed the examination in **First Class with Distinction**.

20.2 Candidate who qualifies for the award of the Degree (vide clause 13) having passed the examination in all the courses within the specified maximum number of semesters (vide clause 2.1), securing a **CGPA not less than 6.5** shall be declared to have passed the examination in **First Class**.

20.3 All other candidates (not covered in clauses 20.1 and 20.2) who qualify for the award of the degree (vide Clause 19) shall be declared to have passed the examination in **Second Class**.

## **21. PROVISION FOR WITHDRAWAL FROM END-SEMESTER EXAMINATION**

21.1 A candidate due to valid reason on prior application may be granted permission to withdraw from appearing for the examination of any one course or consecutive examinations of more than one course in a semester examination.

21.2 Such withdrawal shall be permitted only once during the entire period of study of the degree programme.

21.3 Withdrawal of application is valid only if it is made within 10 days prior to the commencement of the examination in that course or courses and recommended by the HoD / Dean concerned and approved by the Registrar.

21.3.1 Notwithstanding the requirement of mandatory TEN days notice, applications for withdrawal for special cases under extraordinary conditions will be considered on the merit of the case.

- 21.4 Withdrawal shall not be construed as an appearance for the eligibility of a candidate for First Class with Distinction. This provision is not applicable to those who seek withdrawal during IV semester.
- 21.5 Withdrawal from the End semester examination is **NOT** applicable to arrears courses of previous semesters.
- 21.6 The candidate shall reappear for the withdrawn courses during the examination conducted in the subsequent semester.

## **22. PROVISION FOR AUTHORISED BREAK OF STUDY**

- 22.1 **Break of Study shall be granted only once for valid reasons for a maximum of one year during the entire period of study of the degree programme.** However, in extraordinary situation the candidate may apply for additional break of study not exceeding another one year by paying prescribed fee for break of study. If a candidate intends to temporarily discontinue the programme in the middle of the semester for valid reasons, and to rejoin the programme in a subsequent year, permission may be granted based on the merits of the case provided he / she applies to the Registrar, but not later than the last date for registering for the end semester examination of the semester in question, through the HoD stating the reasons therefore and the probable date of rejoining the programme.
- 22.2 The candidate thus permitted to rejoin the Programme after the break shall be governed by the Curriculum and Regulations in force at the time of rejoining. Such candidates may have to do additional courses as per the Regulations in force at that period of time.
- 22.3 The authorized break of study (for a maximum of one year) will not be counted for the duration specified for passing all the courses for the purpose of classification. (Vide Clause 20). However, additional break of study granted will be counted for the purpose of classification.



- 22.4 The total period for completion of the Programme reckoned from, the commencement of the first semester to which the candidate was admitted shall not exceed the maximum period specified in clause 2.1 irrespective of the period of break of study (vide clause 22.3) in order that he/she may be eligible for the award of the degree.
- 22.5 If any student is detained for want of requisite attendance, progress and good conduct, the period spent in that semester shall not be considered as permitted 'Break of Study' or 'Withdrawal' (Clause 21 and 22) is not applicable for this case.

### **23. RANKING**

A candidate who qualifies for the PG Degree programme passing all the Examinations in the first attempt, within the minimum period prescribed for the programme of study from Semester I through Semester IV to the programme shall be eligible for ranking. Such ranking will be confined to 10% of the total number of candidates qualified in that particular programme of Study subject to a maximum of 10 ranks.

**The improved marks will not be taken into consideration for ranking.**

### **24. SUPPLEMENTARY EXAMINATION**

Supplementary Examination will be conducted only for the final semester students within ten days from the date of publication of results for students who have failed in one theory course only. Such students shall apply with prescribed fee to the Controller of Examinations within the stipulated time.

### **25. DISCIPLINE**

25.1. If a student indulges in malpractice in any of the Internal / External Examinations he / she shall be liable for punitive action as prescribed by the KAHE from time to time.

25.2. Every student is required to observe discipline and decorous behavior both inside and outside the campus and not to indulge in any activity which will tend to bring down the prestige of the KAHE. The erring students will be referred to the disciplinary committee constituted by the KAHE, to enquire into acts of indiscipline and recommend the disciplinary action to be taken.

### **26. REVISION OF REGULATION AND CURRICULUM**

Karpagam Academy of Higher Education may from time to time revise, amend or change the Regulations, Scheme of Examinations and syllabi if found necessary.

**DEPARTMENT OF CHEMISTRY**

**FACULTY OF ARTS, SCIENCE AND HUMANITIES**

**PG PROGRAM (CBCS)**

**M.Sc. Chemistry (2021-2022 Batch and onwards)**

Course code	Name of the course	Objectives & Outcomes		Instruction hours per week			Credits	Maximum Marks			Page No.
		PE O's	PO's	L	T	P		CIA	ESE	Total	
<b>Semester-I</b>											
21CHP101	Organic Chemistry - I (Reaction Mechanisms)	1,2,3	a,c,e	4	0	0	4	40	60	100	23
21CHP102	Inorganic Chemistry - I (Nuclear Chemistry and Metallic Clusters)	1,2,3	a,c,e	4	0	0	4	40	60	100	26
21CHP103	Physical Chemistry- I (Quantum Chemistry and Surface Chemistry)	1,2,3	a,c,e	4	0	0	4	40	60	100	29
21CHP104	Organic and Inorganic Spectroscopy	1,2,3,4	a,b,c,h,j	4	0	0	4	40	60	100	32
21CHP105A	Green Chemistry	1,2,3	a,c,e	4	0	0	4	40	60	100	34
21CHP105B	Medicinal Chemistry										36
21CHP105C	Molecular Modelling & Drug Design										38
21CHP111	Organic Chemistry Practical-I (Qualitative Analysis and Single Stage Preparations)	3,4	b,h,j	0	0	4	2	40	60	100	40
21CHP112	Organic Chemistry Practical-II (Quantitative Analysis and Double Stage Preparations)	3,4	b,h,j	0	0	4	2	40	60	100	42
	Journal Paper Analysis & Presentation	1,2,3	a,b,c,d,e,h,j	2	-	-	-	-	-	-	
	<b>Semester Total</b>			<b>22</b>	<b>0</b>	<b>8</b>	<b>24</b>	<b>280</b>	<b>420</b>	<b>700</b>	
<b>Semester-II</b>											
21CHP201	Organic Chemistry-II (Rearrangements, Reactions, Photochemistry and Pericyclic Reactions)	1,2,3	a,c,e	4	0	0	4	40	60	100	44

21CHP202	Inorganic Chemistry-II (Co-ordination Chemistry)	1,2, 3	a,c, e	4	0	0	4	40	60	100	47
21CHP203	Physical Chemistry II (Group Theory & Chemical Kinetics)	1,2, 3	a,c, e	4	0	0	4	40	60	100	50
21CHP204	Instrumental Methods of Chemical Analysis	3,4	f,h	4	0	0	4	40	60	100	53
21CHP205A	Catalysis	1,2, 3	a,c, e	4	0	0	4	40	60	100	55
21CHP205B	Industrial Organic Synthesis										57
21CHP205C	Advanced Energy Storage										59
21CHP211	Inorganic Chemistry Practical-I (Qualitative Analysis and Preparations)	3,4	b,h,j	0	0	4	2	40	60	100	61
21CHP212	Inorganic Chemistry Practical-II (Quantitative Analysis and Complex Preparations)	3,4	b,h,j	0	0	4	2	40	60	100	63
	Journal Paper Analysis & Presentation	1,2, 3	a,b, c,d, e,h,j	2	-	-	-	-	-	-	
	Internship	-	-	-	-	-	-	-	-	-	
	<b>Semester Total</b>			<b>22</b>	<b>0</b>	<b>8</b>	<b>24</b>	<b>280</b>	<b>420</b>	<b>700</b>	
<b>Semester-III</b>											
21CHP301	Organic Chemistry- III (Natural Products)	1,2, 3	a,c, e	4	0	0	4	40	60	100	65
21CHP302	Physical Chemistry-III (Thermodynamics)	1,2, 3	a,c, e	4	0	0	4	40	60	100	67
21CHP303	Physical Methods in Chemistry (Instrumentation)	1,2, 3	a,c, e	4	0	0	4	40	60	100	70
21CHP304	Nanochemistry	3,4	f,h	4	0	0	4	40	60	100	72
21CHP305A	Polymer Chemistry	1,2, 3	a,c, e	4	0	0	4	40	60	100	74
21CHP305B	Textile Chemistry										76
21CHP305C	Industrial Chemistry										78
21CHP311	Physical Chemistry Practical-I (Molecular Weight Determination and Conductometric Titrations)	3,4	b, h,i	0	0	4	2	40	60	100	80
21CHP312	Physical Chemistry Practical-II (Chemical Kinetics and Potentiometric Titrations)	3,4	b, h,i	0	0	4	2	40	60	100	82
	Journal Paper Analysis & Presentation	1,2, 3	a,b, c,d, e,h,j	2	-	-	-	-	-	-	
	<b>Semester Total</b>			<b>22</b>	<b>0</b>	<b>8</b>	<b>24</b>	<b>280</b>	<b>420</b>	<b>700</b>	

**Semester-IV**

21CHP419	Project and Viva-Voce	1,2,3	ab,c,d,e,h,j	-	-	30	15	80	120	200	84
<b>Semester Total</b>				<b>0</b>	<b>0</b>	<b>30</b>	<b>15</b>	<b>80</b>	<b>120</b>	<b>200</b>	
<b>Grand Total</b>				<b>66</b>	<b>0</b>	<b>54</b>	<b>87</b>	<b>920</b>	<b>1380</b>	<b>2300</b>	

**List of Core Course Elective**

<b>Elective-I</b>		<b>Elective-I</b>		<b>Elective-III</b>	
<b>Code</b>	<b>Course</b>	<b>Code</b>	<b>Course</b>	<b>Code</b>	<b>Course</b>
21CHP105A	Green Chemistry	21CHP205A	Catalysis	21CHP305A	Polymer Chemistry
21CHP105B	Medicinal Chemistry	21CHP205B	Industrial Organic Synthesis	21CHP305B	Textile Chemistry
21CHP105C	Molecular Modelling & Drug Design	21CHP205C	Advanced Energy Storage	21CHP305C	Industrial Chemistry

### **Programme Outcomes (PO's)**

- a. Students will have a firm foundation in the fundamentals and application of current chemical and scientific theories including those in Analytical, Inorganic, Organic and Physical Chemistries.
- b. Students will be able to design and carry out scientific experiments as well as accurately record and analyze the results of such experiments.
- c. Students will be skilled in problem solving, critical thinking and analytical reasoning as applied to scientific problems.
- d. Students will be able to clearly communicate the results of scientific work in oral, written and electronic formats to both scientists and the public at large.
- e. Students will be able to explore new areas of research in both chemistry and allied fields of science and technology.
- f. Students will appreciate the central role of chemistry in our society and use this as a basis for ethical behavior in issues facing chemists including an understanding of safe handling of chemicals, environmental issues and key issues facing our society in energy, health and medicine.
- g. Students will be able to function as a member of an interdisciplinary problem solving team.
- h. The graduate has specific skills in planning and conducting advanced chemical experiments and applying structural-chemical characterisation techniques.
- i. Are able to use modern instrumentation and classical techniques, to design experiments, and to properly record the results of their experiment.
- j. Are able to use modern library searching and retrieval methods to obtain information about a topic, chemical, chemical technique, or an issue relating to chemistry.

### **Programme Specific Outcomes (PSO's)**

- k. A graduate with a Master's degree in Chemistry has in-depth and detailed functional knowledge of the fundamental theoretical concepts and experimental methods of chemistry.
- l. Students should have an advanced level understanding of the following areas of chemistry - Analytical, Inorganic, Organic, and Physical Chemistry. They should master graduate level understanding of their major area(s) of research.
- m. Students should be able to communicate scientific results in writing and in oral presentation.
- n. Students should become proficient in their specialized area of chemistry and acquire the basic tools needed to carry out independent chemical research.

### Programme Educational Objectives PEO-1

The Masters in Chemistry will extend your depth and breadth of knowledge in all branches of chemistry, suitable for a professional chemist capable of conducting research.

### PEO-2

To carryout research in the trust areas of chemistry. Will be able to communicate effectively the scientific information and research results in written and oral formats, to both professional scientists and to the public.

### PEO-3

To motivate critical thinking and analytical skills to solve complex chemical problems and the Ability to handle problems of practical relevance to society while complying with economical, environmental, ethical, and safety factors.

### PEO-4

To practice chemistry by performance of experiments in the laboratory classes. To perform accurate quantitative measurements with an understanding of the theory and use of contemporary chemical instrumentation, interpret experimental results, perform calculations on these results and draw reasonable, accurate conclusions

### Mapping

PO	a	b	c	d	e	f	g	h	i	j	k	l	m	n
PEO 1	x	x			x			x	x		x	x	x	
PEO 2		x	x	x	x			x	x		x		x	x
PEO 3			x	x		x	x			x			x	x
PEO 4	x	x	x			x		x		x	x	x		x

21CHP101

**ORGANIC CHEMISTRY- I  
(REACTION MECHANISMS)****Semester-I  
4H 4C****Instruction Hours/week: L: 4 T: 0 P: 0 Marks: Internal: 40 External: 60 Total: 100  
External Semester Exam: 3 Hrs****Course Objectives**

This course enables the students to

- Understand aromaticity.
- Know about different name reactions and their application in synthesis.
- Learn addition and elimination reactions.
- Gain knowledge about reaction intermediates.
- Illustrate the principles and reaction mechanisms involving various electrophilic and nucleophilic, addition and elimination reactions.
- Compare and contrast the different organic reaction mechanisms.

**Course Outcomes (CO's)**

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

1. Learn the concept aromaticity and various types of aromaticity
2. Familiarize the various types of electrophilic and nucleophilic substitution reactions and their mechanism.
3. Learn the familiar addition and elimination reactions
4. Describe the concept of reaction intermediates.
5. Understood about the synthesis of aromatic compounds using electrophilic and nucleophilic substitution, addition and elimination reactions.
6. Explain the various organic reaction mechanisms.

**UNIT - I Aromaticity and chemical methods in mechanisms**

Aromaticity-introduction-Modern definitions of aromaticity, Huckel's rule & Craig's rule-aromaticity of benzenoid and heterocyclic compounds. Non-benzenoid aromatics-annulenes, azulenes, ferrocenes and fulvenes.

Kinetic and non-kinetic methods of study of reaction mechanisms - kinetic methods-Primary and secondary kinetic isotopic effects. Non-kinetic methods-study of intermediates, isotopic labeling, stereochemical studies, energy profile diagrams and cross over experiments. Hammond's postulate. Kinetic and thermodynamic control.

Linear free energy relationship - Hammett equation and Taft equation.

## **UNIT - II Addition reactions and Concepts in organic synthesis**

Electrophilic, nucleophilic and free radical addition to double and triple bonds- hydration, hydroxylation, Michael addition, hydroboration and epoxidation.

Addition reactions to carbonyl compounds – Mannich reaction, Meerwein Ponderoff- Verley reduction, Grignard, Claisen, Dieckmann, Stobbe, Knoevenagel, Darzen, Wittig, Thorpe and Benzoin reactions.

**Concepts in organic synthesis:** An introduction to Retrosynthesis, types of synthesis- linear and convergent synthesis.

## **UNIT - III Electrophilic substitution reactions**

Aromatic electrophilic substitution reactions-formylations–Gattermann, Gattermann Koch, Riemer Tiemann and Vilsmeier-Haack reactions. Kolbes, Bischler-Napieralski and Hofmann-Martius reactions. Friedel crafts alkylation and acylations.

Aliphatic electrophilic substitution reactions - mechanisms- SE1, SE2 and SEi - structure reactivity relationship, typical electrophilic substitution reactions - Friedel crafts acylation at olefinic carbon, Stork enamine reaction and decarboxylation of aliphatic acids.

## **UNIT - IV Nucleophilic substitution reactions**

Aliphatic nucleophilic substitution reactions- mechanisms - S<sub>N</sub>1, S<sub>N</sub>2, ion pair and S<sub>N</sub>i- substitution at vinyl carbon. Stereochemistry of nucleophilic substitution reaction - effect of substrate structure - solvent effects - leaving group effect – nucleophilicity, ambident nucleophiles and ambident substrates- neighbouring group participation.

Aromatic nucleophilic substitution reactions - benzyne mechanism, intermediate complex mechanism and S<sub>N</sub>1 mechanism, structure reactivity relationship.

Ziegler alkylation and Chichibabin reaction.

## **UNIT - V Elimination reactions and Reagents in organic synthesis**

**Elimination reactions:** E1, E2, Ei and E1cB mechanisms - stereochemistry of eliminations. Hofmann rule-Saytzeff rule-Bredts rule– Substitution versus Elimination. Typical elimination reaction - Chugaev reaction, Hofmann degradation and Cope elimination.

Carbenes and nitrenes-structure, generation and reactions.



**Reagents in organic synthesis:** Preparations and synthetic applications of DDQ, DBU, Dimethyl sulfoxide, trimethyl silyl iodide, Osmium tetroxide, Selenium dioxide, Dicyclohexylcarbodiimide (DCC), LDA, DIBAL-H and Mercuric acetate.

### SUGGESTED READINGS

1. Smith, M. B. (2015). *March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure* (VII Edition). New Jersey: John Wiley & Sons, Inc., Hoboken.
2. Peter Sykes, (1995). *A guidebook to mechanism in Organic Chemistry* (VI Edition). New York: John Wiley & sons Inc.
3. Sanyal, S. N. (2014). *Reactions, Rearrangements and Reagents* (IV Edition). New Delhi: Bharathi Bhawan (Publishers and Distributors).
4. Tewari, N. (2011). *Advanced Organic Reaction Mechanism* (III Edition). Kolkata: Books and Allied (P) Ltd.
5. Warren, S., & Wyatt, P. (2008). *Organic Synthesis: The Disconnection Approach* (II Edition). John Wiley & Sons Ltd., Chichester.
6. Clayden, J., Greeves, N. & Warren, S. (2012). *Organic Chemistry* (II Edition). Oxford University Press, Oxford.

21CHP102

**INORGANIC CHEMISTRY-I  
(NUCLEAR CHEMISTRY AND METALLIC CLUSTERS)****Semester-I  
4H 4C****Instruction Hours/week: L: 4 T: 0 P: 0 Marks: Internal: 40 External: 60 Total: 100  
External Semester Exam: 3 Hrs****Course Objectives**

This course enables the students to

- Understand the nuclear structure, stable and unstable atomic nuclei, nuclear reactions and different modes of radioactive decay and also methods for measurements of radioactivity.
- Analyze the various defects and its application on inorganic crystals.
- Understand the detection of radioactive rays and to measure the radiation.
- Learn about the fundamentals of metallic clusters.
- Understand the chemistry of boranes and related compounds.
- Apply the knowledge to know about the various forms of inorganic compounds.

**Course Outcomes (CO's)**

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

1. Describe the basic concepts of nuclear chemistry and types of nuclear reactions.
2. Discriminate various defects and also known their application on inorganic crystals.
3. Understood the basics of metallic clusters, preparation, properties and applications of metallic clusters.
4. Analyse the structure and bonding in molecules / ions and predict the structure of molecules / ions.
5. Describe the type of defects in metals and about semi conductors.
6. Understood the inorganic and organometallic chemistry, catalysis in the molecular level.

**UNIT - I Inorganic Rings, Cages and Clusters**

Inorganic chains – rings - cages and clusters (definition and structure) - metal clusters - dinuclear clusters - trinuclear clusters - tetranuclear clusters - hexanuclear clusters - organometallic clusters. Silicates and siloxanes. Fullerenes and their similar compounds.

Boranes, boron hydrides (structure and properties) – carboranes - metallocarboranes - Wade's theory -closo-nido and arachno structures - borazines, phosphazenes - Sulphur-Nitrogen ring compounds. Isopoly and heteropoly acids of V, Cr, Mo and W.

## **UNIT - II Metallic State and Organometallic chemistry**

Metallic state-free electron, band and zone theories - non stoichiometry - point defects in solids - Schottky and Frenkel defects - linear effects - dislocation - effects due to dislocation - electrical properties of solids - insulators-intrinsic semiconductors - n and p type and super conductors - ceramics elementary treatment.

Basic Organometallic Chemistry: Common notation used in organometallic chemistry- Metal-ligand interactions; Basic principles of ligand-field theory; molecular orbital theory - 18-electron rule - Common organometallic bonding modes – Introduction to Metal-centered organometallic reactions.

## **UNIT - III Heterogenous catalytic reactions**

Organometallic compounds in homogeneous catalytic reactions-coordinative unsaturation – acid-base behavior reaction–migration of atoms or groups from metal to ligand–insertion reaction–reactions of coordinated ligands–catalytic reactions of alkenes–isomerisation of alkenes – hydrogenation– hydroformylation and hydrosilation of alkenes – alkene polymerization and oligomerisation – fluxional molecules.

## **UNIT - IV Nuclear Chemistry**

Nuclear Chemistry - the nucleus - subatomic particles and their properties, binding energy. N/P ratios in stable and meta stable nuclei - different type of nuclear forces - liquid model-shell model. Modes of radioactive decay -  $\alpha$ ,  $\beta$  and  $\gamma$  decay radiation, electron capture, nuclear isomerism and internal conversion. Thermo nuclear reactions.

## **UNIT - V Nuclear Reactions**

Nuclear reactions - Bethes's notation, Q-value, columbic barrier, cross section, different types of nuclear reactions - projectiles capture - particle emission, spallation, fission, fusion, theories of fission, use of fission products, nuclear reactors - fissile and fertile isotopes-  $U^{233}$ ,  $U^{235}$ ,  $Pu^{239}$ ,  $Th^{232}$ , -atomic power projects in India, stellar energy, synthetic elements - application of radio isotopes - Hot atom chemistry.

## **SUGGESTED READINGS**

1. Huheey, J. E., Keitler, E. A., & Keitler, R. L. (2011). Inorganic Chemistry- Principles of Structure and Reactivity (IV Edition). Singapore: Pearson Education.
2. Shekar, C. V. (2014). A Text Book of Nuclear Chemistry (I Edition). New Delhi: Dominant publishers and Distributors (P) Ltd.
3. Arnikar, H. J. (2011). Essentials of Nuclear Chemistry (IV Edition). New Delhi: New Age International Publishers Pvt. Ltd.
4. B. D. Gupta. (2013). Basic Organometallic Chemistry: Concepts, Syntheses and Applications. Universities Press.
5. Cotton, F. A., Wilkinson, G., Murillo, C. A., & Bochmann, M. (1999). Advanced Inorganic Chemistry (VI Edition). New York: John Wiley & Sons.

6. Glasstone, S. (2014). Sourcebook on Atomic Energy (III Edition). New Delhi: East West Press.
7. Gurdeep Raj, (2014). Advanced Inorganic Chemistry Vol. I (24<sup>th</sup> Revised Edition). Meerut: Goel Publishing House.
8. Madan, R. D. (2019). Modern Inorganic Chemistry. New Delhi: S. Chand & Co.
9. Puri, B. R., Sharma, L. R. & Kalia, K. C. (2017). Principles of Inorganic Chemistry (33<sup>rd</sup> Edition). New Delhi: Shoban Lal & Co.
10. Malik, W. C., Tuli, G.D. & Madan. R.D. (2010). Selected topics in Inorganic Chemistry. New Delhi. S. Chand & Co.

21CHP103

**PHYSICAL CHEMISTRY- I**  
**(QUANTUM CHEMISTRY AND SURFACE CHEMISTRY)****Semester-I**  
**4H 4C****Instruction Hours/week: L: 4 T: 0 P: 0 Marks: Internal: 40 External: 60 Total: 100**  
**External Semester Exam: 3 Hrs****Course Objectives**

This course enables the students to

- Remember the fundamentals and applications of classical mechanics and quantum chemistry.
- Understand the structure of an atom and different approximation methods.
- Understand the concept of surface chemistry and their applications.
- Apply the molecular phenomena and its model problems.
- Analyse the probabilities, amplitudes, averages, expectation values and observables.
- Understand the basic principles of surface chemistry and their applications.
- Evaluate the different theories of adsorption and catalysis.

**Course Outcomes (CO's)**

On the completion of this course, Students should have to

1. Differences between classical and quantum mechanics and the limitations of classical mechanics.
2. Describe about the connection of quantum mechanical operators to observables probabilities, amplitudes, averages, expectation values, and observables.
3. Discuss the molecular phenomena can be related to model problems.
4. Differentiate between common approximation methods and standard chemical frameworks (Born-Oppenheimer approximation, molecular orbitals, examples)
5. Differentiate different theories of adsorption and catalysis.
6. Understood the basic principles of surface chemistry and their applications.

**UNIT - I Failure of classical mechanics and Operators**

Failure of classical mechanics and the success of quantum theory in explaining black body radiation and photoelectric effect.

The time dependent and time independent Schrodinger equations - Born's interpretation of the wave function. Requirements of the acceptable wave function.

Algebra of operators. Sums and products of operators - commutator - linear operators- eigen functions and eigen values - correspondence between physical quantities in classical mechanics and operators in quantum mechanics - Hamiltonian operator - angular momentum operator. Quantization of angular momentum and its spatial orientation - average values - postulates of quantum mechanics.

## **UNIT - II Schrodinger equation**

Particle in a one-dimensional box - quantization of energy - normalization of wave function - orthogonality of the particle in a one-dimensional box wave functions. Illustration of the uncertainty principle and correspondence principle with reference to the particle in a one-dimensional box - particle in a three dimensional box - separation of variables.

Solving of Schrodinger equation for one-dimensional harmonic oscillator. Harmonic oscillator model of a diatomic molecule. Illustration of the uncertainty principle and correspondence principle with reference to harmonic oscillator. Solving of Schrodinger equation for a rigid rotor. Rigid rotor model of a diatomic molecule.

## **UNIT - III Approximation Methods**

Schrodinger equation for the H-atom (or H-like species)- separation of variables - energy levels. Radial distribution functions - orbitals and orbital shapes. Probability density and radial distribution functions.

Need for approximation methods. The perturbation theory- application of perturbation method to systems such as anharmonic oscillator and He-atom.

The variation method - application of variation method to systems such as anharmonic oscillator and He-atom.

## **UNIT - IV Surface Chemistry-I**

Adsorption and free energy changes at interfaces-Solid-gas interface-Langmuir, BET isotherms-Surface area determination-soluble and insoluble film-Solid - liquid interfaces-Gibbs adsorption isotherm-contact angle and wetting-applications of adsorption.

Role of surface in catalysis-semiconductor catalysis-n and p-type surfaces. Specific and general acid base catalysis: Bronsted catalysis law-Hammett acidity functions. Enzyme catalysis: Michaelis Menten Law- Influence of pH and temperature on enzyme catalysis.

Heterogeneous catalysis: Kinetics of bimolecular surface reactions-Langmuir-Hinshelwood mechanism, Langmuir Rideal mechanism and Rideal-Eley mechanism.

## **UNIT - V Surface Chemistry-II**

Electrical aspects of surface chemistry-theories of electrical double layers Helmholtz, Gouy chapmann and Stern theories. Zeta potential concept, determination and applications, electrophoresis, electroosmosis, sedimentation and streaming potential- micelles and reverse micelles, micro emulsions.

Principle, instrumentation and applications of ESCA, SERS and Auger spectroscopy.

## SUGGESTED READINGS

1. Prasad, R. K. (2014). Quantum Chemistry (IV Revised Edition). New Delhi: New Age International Publishers Pvt. Ltd.
2. Chandra, A. K. (2017). Quantum Chemistry (IV Edition). New Delhi: Tata McGraw – Hill Publishing Company Ltd.
3. House, J. E. (2004). Fundamental of Quantum Chemistry (II Edition). New Delhi: Academic Press.
4. Levine, I. N. (2016). Quantum Chemistry (VII Edition). New Delhi: Pearson Education Pvt. Ltd.
5. Puri, B. R., Sharma, L. R., & Pathania, M. S. (2013). Principles of Physical Chemistry (46<sup>th</sup> Edition). Jalandar: Vishal Publishing Co.
6. Atkins, P., & De Paula, J. (2014). Atkins Physical Chemistry (X Edition). Oxford: Oxford University Press.

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21CHP104	ORGANIC AND INORGANIC SPECTROSCOPY	Semester-I 4H 4C
Instruction Hours/week: L: 4 T:0 P:0		Marks: Internal: 40 External: 60 Total: 100
External Semester Exam: 3 Hrs		

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**Course Objective**

This course enables the students to

- Learn knowledge about electronic spectroscopy.
- Understand about IR spectroscopy.
- Understand the basic concept of NMR spectroscopy
- Apply the different aspects of NMR spectroscopy to predict the structure of compounds.
- Analyze about the mass spectroscopy and mossbauer spectroscopy.
- Evaluate about the invaluable tools in synthetic chemistry for the confirmation of known molecules and elucidation of shape and structures of unknown compounds of high complexity with a high degree of certainty.

**Course Outcomes (CO's)**

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

1. Recognize the basic concepts of electronic and IR spectroscopy.
2. Understand the valuable concepts in NMR spectroscopy.
3. Discuss the basic knowledge about mass spectroscopy.
4. Explore the different aspects of NMR spectroscopy to predict the structure of compounds.
5. Differentiate the mass and mossbauer spectroscopy
6. Predict the structure of unknown molecules by using the spectral data and to identify the structure of the molecules.

**UNIT - I Ultraviolet and Visible Spectroscopy**

Electronic spectra of diatomic molecules - laws of photochemistry - electronic absorption transitions-correlation of electronic structure with molecular structure - simple chromophoric groups - effects of conjugation - Woodward -Fisher rules for  $\alpha$ ,  $\beta$  unsaturated carbonyl compounds & dienes - aromatic systems with extended conjugation - applications to organic and inorganic compounds - Instrumentation.

**UNIT - II Infrared Spectroscopy**

The vibrating diatomic molecules-the simple harmonic oscillator and anharmonic oscillator - the diatomic rotor - factors influencing vibrational frequencies - identification of fundamental groups. Fingerprint region-application to organic and inorganic compounds-Instrumentation.



### **UNIT - III NMR Spectroscopy**

Principle of NMR spectroscopy – description of the PMR instrument, factors affecting chemical shifts-chemical shift equivalence and magnetic equivalence - spin-spin coupling - first order and non-first order spectra - Hetero nuclear coupling in  $^1\text{H}$ NMR - deuterium exchange - high field spectra - double resonance-shift reagents-applications to organic and inorganic compounds.

FT NMR.  $^{13}\text{C}$  NMR spectroscopy-factors affecting the chemical shifts - broad band and off-resonance decoupling - applications in organic chemistry. 2D-NMR- Correlation spectroscopy-  $^1\text{H}$ - $^1\text{H}$  COSY,  $^1\text{H}$ - $^{13}\text{C}$  HETEROCOSY and DEPT techniques.

### **UNIT - IV Mass Spectroscopy**

Principles of mass spectrometry – resolution - description of single focusing and double focusing electron impact mass spectrometers - presentation and analysis of spectra - determination of molecular formulae - Nitrogen rule- Stevenson's rule - isotope abundance analysis - meta stable ions and peaks the molecular ion peak - fragmentation processes - Retro Diels - Alder rearrangement - McLafferty rearrangement - ortho effect - fragmentation associated with functional groups - aldehydes, ketones, carboxylic acids, esters, amides, alcohols, thiols, amine, ethers, sulphides and halides..

### **UNIT - V Mossbauer & Problems**

Mossbauer spectroscopy – principles - spectrometer - isomer shift - quadrapole interaction - nuclear Zeeman splitting – applications.

Problems involving UV, IR, NMR, Mass spectral data (for compounds not more than 10 carbon atoms).

### **SUGGESTED READINGS**

1. Jag Mohan. (2018). Organic Spectroscopy: Principles and Applications (II Edition). New Delhi: Narose Publishing House.
2. Kemp, W. (2017). Organic Spectroscopy (III Edition). New York: Palgrave Macmillan.
3. Sharma, Y. R. (2013). Elementary Organic Spectroscopy: Principles and Chemical Applications (Revised V Edition). New Delhi: S. Chand & Company Limited.
4. Silverstein, R. M., Webster, F. X., & Kiemle, D. (2014). Spectroscopy of Organic Compounds (VIII Edition). New York: John Wiley & Sons.
5. Levine, I. N. (2013). Quantum Chemistry (VII Edition). New Delhi: Pearson Education Pvt. Ltd.
6. Drago, R.S. (2012). Physical Methods in Inorganic Chemistry. New York: East- West Press Pvt. Ltd.
7. Banwell.,(2017). Fundamentals of Molecular & Spectroscopy (IV Edition), McGraw-Hill Education (India) Pvt. Limited

21CHP105A

GREEN CHEMISTRY

Semester-I

4H 4C

**Instruction Hours/week: L: 4 T:0 P: 0 Marks: Internal: 40 External: 60 Total: 100**  
**External Semester Exam: 3 Hrs**

### Course Objectives

This course enables the students to

- Gain knowledge about the concept of Green chemistry.
- Understand the basics of Green chemistry.
- Analyze the 12 principles of Green chemistry as well as the tools of Green chemistry.
- Apply how to evaluate a reaction or process and determine “Greener” alternatives.
- Focus on the application of greener routes to improve industrial processes and to produce important products.
- Evaluate the greener synthetic pathway to produce pharmacological compounds.

### Course Outcomes (CO’s)

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

1. Design chemical products and processes that reduce or eliminate the use and generation of hazardous substances.
2. Create awareness for reducing waste, minimizing energy consumption in organic synthesis.
3. Explain the techniques of green synthesis in organic reactions.
4. Relate the various alternative resources for green technology in organic synthesis.
5. Demonstrate various greener synthetic pathways and implement it in the production of pharmacological compounds.
6. Evaluate the concept of microwaves and ionic liquids in various chemical reactions.

### UNIT - I Introduction to Green Chemistry and Principles of Green Chemistry

What is Green Chemistry? Need for Green Chemistry. Goals of Green Chemistry. Limitations/ Obstacles in the pursuit of the goals of Green Chemistry. Twelve principles of Green Chemistry with their explanations.

### UNIT - II Designing a Green Chemical synthesis

Designing a Green synthesis using these principles: prevention of waste/by products; maximum incorporation of the materials used in the process into the final products, atom economy, and calculation of atom economy of the rearrangement, addition, substitution and elimination reactions. Green solvents– supercritical fluids, water as a solvent for organic reactions, ionic liquids, fluorous biphasic solvent, PEG, solvent less processes, immobilized solvents and how to compare greenness of solvents.

### **UNIT - III Alternative sources of Energy**

Energy requirements for reactions – alternative sources of energy: use of microwaves and ultrasonic energy. Microwave assisted reactions in water: Hofmann elimination, methyl benzoate to benzoic acid, oxidation of toluene and alcohols; microwave assisted reactions in organic solvents. Diels-Alder reaction and decarboxylation reaction. Ultrasound assisted reactions: sono chemical Simmons-Smith Reaction (Ultrasonic alternative to iodine).

### **UNIT - IV Green synthesis/reaction**

Green starting materials, Green reagents, Green solvents, reaction conditions, Green catalysis and Green synthesis- Real world cases (Traditional processes and green ones) Synthesis of Ibuprofen, Adipic acid, disodium iminodiacetate (alternative to Strecker synthesis).

### **UNIT - V Hazard assessment and mitigation in chemical industry**

Future trends in Green Chemistry-oxidation-reduction reagents and catalysts; biomimetic, multifunctional reagents; Combinatorial green chemistry; Proliferation of solventless reactions; Noncovalent derivatization. Biomass conversion, emission control and biocatalysis.

### **SUGGESTED READINGS**

1. Ahluwalia, V. K., & Kidwai, M. (2012). *New Trends in Green Chemistry* (II Edition). Germany: Kluwer Academic Publisher.
2. Anastas, P. T., & Warner, J. C. (1998). *Green Chemistry: Theory and Practice*. Oxford: Oxford University Press.
3. Matlack, A. S. (2001). *Introduction to Green Chemistry*. New York: Marcel Dekker.
4. Cann, M. C., & Connely, M. E. (2000). *Real-World cases in Green Chemistry*. Washington: American Chemical Society.
5. Ryan, M. A., & Tinnesand, M. (2002). *Introduction to Green Chemistry*, Washington: American Chemical Society.
6. Lancaster, M. (2010). *Green Chemistry: An Introductory Text* (II Edition). Cambridge: RSC Publishing.
7. Clark, J. H, & Macquarrie, D. J. (2002). *Handbook of Green Chemistry & Technology*. Abingdon: Blackwell Publishing.

21CHP105B

MEDICINAL CHEMISTRY

Semester-I  
4H 4C

Instruction Hours/week: L: 4 T:0 P: 0 Marks: Internal: 40 External: 60 Total: 100  
External Semester Exam: 3 Hrs

**Course Objectives**

This course enables the students to

- Understand the basics of medicinal chemistry.
- Gain knowledge on drug targets, drug metabolism and clinical training.
- Understand the in-silico techniques involved in drug development.
- Discussion about membrane and receptors in drug delivery process.
- Apply the various theoretical laws to predict the pharmaco-kinetics of the compounds.
- Analyze the molecular receptor binding and molecular recognition of the natural and synthetic compounds.

**Course Outcomes (CO's)**

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

1. Understand the basics of medicinal chemistry.
2. Describe the drug targets, drug metabolism and about clinical training.
3. Associate the in-silico techniques involved in drug development.
4. Discuss about the membrane and receptors in drug delivery process.
5. Apply various theoretical laws to predict the pharmaco-kinetics of the compounds.
6. Compare the molecular receptor binding and molecular recognition of the natural and synthetic compounds.

**UNIT - I Drug discovery, design and development**

Synthesis of the representative drugs of the following classes: analgesic, antipyretic and anti-inflammatory agents (Aspirin, paracetamol and Ibuprofen); antibiotics (Chloramphenicol); antibacterial agents (Sulphonamides), antiviral agents (Acyclovir), Central Nervous System agents (Phenobarbital and Diazepam).

**UNIT - II Insilco Drug Design and Computer Assisted New Lead Design**

Introduction, historical perspective, drug compounds, preparation and organization for drug seeking, common stages in the drug seeking campaign, sources of hits, leads and candidate drugs, natural products: higher plant and animal products, combinational libraries, lead optimization. Introduction, basic concepts, molecular recognition by receptor and ligand design, active conformation, approaches to discover new functions, approaches to the cases with known and unknown receptor structure and molecular docking study. Introduction to drug metabolism, toxicity and pharmacokinetics, toxicology considerations, problems and drawbacks on drug discovery and development.

### **UNIT - III Membranes and Receptors**

Drug transport mechanism and absorption processes, pharmacodynamic and pharmacokinetic aspects, prodrugs and bioactivation, receptor theories and receptor models, drug receptor interactions drug design, physiochemical principles and basis of drug design, different methods of drug design,

### **UNIT - IV QSAR**

Electronic effects; Hammett equation, Lipophilicity effects; Hansch equation, Steric Effects; Taft Equation; Experimental and theoretical approaches for the determination of physico-chemical parameters, parameter inter-dependence; linearity versus non-linearity; The importance of biological data in the correct form; Molecular docking and dynamics: Rigid docking, flexible docking and manual docking.

### **UNIT - V Molecular Recognition in Drug-Receptor Binding**

Molecular forces and binding energetic, enzyme inhibitors - modes of inhibition and general approaches. Antibacterial drugs - major drug classes and drug resistance, antiviral drugs- major drug classes and drug resistance, anticancer drugs- major cancer drug targets, major drug classes and drug resistance.

### **SUGGESTED READINGS**

1. Ahluwalia, V. K. (2012). Green Chemistry-Environmentally Benign Reactions. New Delhi: Ane Books Pvt Ltd.
2. Ghose, J. (2012). A Text book of Pharmaceutical Chemistry. New Delhi: S. Chand Pub Ltd.
3. Ilango, K., & Valentina, P. (2017). Text Book of Medicinal Chemistry. Vol II. Chennai: Keerthi Publishers.
4. Ashutosh Kar, (2018). Medicinal Chemistry (III Edition). New Delhi: New Age International Publishers.
5. Stanley E. Manahan, (2006). Green Chemistry and the Ten Commandments of Sustainability (II Edition). Columbia, Missouri U.S.A: ChemChar Research. Inc Publishers Columbia.
6. Chatterjea, M. N., & Shinde, R. (2012). Textbook of Medicinal Biochemistry. New Delhi: Jaypee Brothers. Medical Publishers (P) Ltd.
7. G.L. Patrick, (2013). Introduction to Medicinal Chemistry (I Edition). UK: Oxford University Press.
8. Mukhopadhyay, R., Patta, S., & Rajib Kumar Das. (2011), Textbook of Pharmaceutical and Medicinal Chemistry. Arunabha Son Publishers.
9. Parimoo, P., (2009). Text book of Medicinal Chemistry. CBS Publishers, New Delhi.

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<b>21CHP105C</b>	<b>MOLECULAR MODELLING &amp; DRUG DESIGN</b>	<b>Semester-I</b>
		<b>4H 4C</b>
<b>Instruction Hours/week:L: 4 T:0 P:0</b>		<b>Marks: Internal: 40 External: 60 Total:100</b>
<b>External Semester Exam: 3 Hrs</b>		

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### Course Objectives

This course enables the students to

- Acquaint with theoretical and practical aspects of molecular modeling tools and techniques for drug design and discovery.
- Analyse molecular modeling software will be useful for drug discovery and developments.
- Perform molecular modelling using the softwares.
- Analyse about the importance of pharmacophores in drug discovery process.
- Predict the physical and biological properties of natural/synthesized molecules.
- Evaluate the drug-receptor binding affinities of the compounds by using in-silico method.

### Course Outcomes (CO's)

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

1. Describe the molecular modeling and field effects as a part of drug discovery.
2. Understand the various stages and various targets of drug discovery.
3. Classify the importance of the pharmacophores in drug discovery.
4. Analyses the importance of the role of computer aided drug design in drug discovery.
5. Practice and predict the physical and biological properties of natural/synthesized molecules.
6. Evaluate the drug-receptor binding affinities of the compounds by using in-silico method.

### UNIT - I Introduction to Molecular Modelling

Introduction to drug design, discovery and development- drug metabolism- toxicity and pharmacokinetics. Useful concepts in molecular modelling: Coordinate systems. Potential energy surfaces, electron density surface. Molecular graphics. Surfaces. Solvent exclude surface and solvent accessible surface. Computer hardware and software. The molecular modelling literature.

### UNIT - II Force Fields for molecular modelling

Fields. Bond stretching. Angle bending, torsional term and miscellaneous interaction. Introduction to nonbonded interactions. Electrostatic interactions. Van der Waals Interactions. Hydrogen bonding in molecular mechanics– parameterization of a force field, anharmonic distributed multiple and polarizable force fields, hydrophobic effect and

solution energy- potential of mean force. Force field models for the simulation of liquid water. Difference between spectroscopy and molecular mechanic force field.

### **UNIT - III Basics of molecular modelling**

Basics of molecular modelling, methods, steps involved in MM, selection of target and template, homology modelling, refinement and validation - SAVES server, the critical assessment of protein structure prediction (CASP), superposition of proteins using different tools, RMSD, presentation of protein conformations, hydrophobicity factor, shape complementary.

**QSAR:** Principles of ligand based drug design SAR, QSAR and 3D QSAR- receptor based drug design - principles of receptor based de novo ligand design- rigid body molecular docking- statistical techniques behind QSAR.

### **UNIT - IV Pharmacophore**

Historical perspective and viewpoint of pharmacophore, functional groups considered as pharmacophores, Ehrlich's "Magic Bullet", Fischer's "Lock and Key", two-dimensional pharmacophores, three-dimensional approach of pharmacophores, criteria for pharmacophore model, pharmacophore model generation software tools, molecular alignments, handling flexibility, alignment techniques, scoring and optimization, pharmacophores, validation and usage, automated pharmacophore generation methods, GRID-based pharmacophore models, pharmacophores for hit identification, pharmacophores for human ADME/tox-related proteins.

### **UNIT - V Computer aided Chemistry: Structure Prediction and Drug Design**

Introduction to molecular docking, rigid docking, Flexible docking, manual docking, advantage and disadvantage of flex-X, flex-S, AUTODOCK and other docking software, scoring functions, simple interaction energies, GB/SA scoring (implicit solvation), C Score (consensus scoring algorithms).

### **SUGGESTED READINGS**

1. Leach, A. R. (2001). Molecular Modelling Principles and Application (II Edition). Longman: Prentice Hall.
2. Haile, J. M. (1997). Molecular Dynamics Simulation Elementary Methods (I Edition). UK: John Wiley and Sons.
3. Gupta, S. P. (2008). QSAR and Molecular Modeling (I Edition). Springer-Netherlands: Anamaya Publishers.

21CHP111

ORGANIC CHEMISTRY PRACTICAL-I

Semester -I

4H 2C

(QUALITATIVE ANALYSIS AND SINGLE STAGE PREPARATIONS)

Instruction Hours/week: L:0 T: 0 P: 4 Marks: Internal: 40 External: 60 Total: 100  
External Semester Exam: 6 Hrs

### Course Objectives

This course enables the students to

- Understand the principles behind the qualitative analysis by semi micro-qualitative analysis method.
- Apply the techniques to prepare of organic compounds.
- Understand the basic concept and advantages of semi- micro qualitative analysis.
- Analyze the systematic separations of organic mixtures.
- Apply the step wise procedure to predict the functional groups present in the organic mixture.
- Evaluate the functional groups with their special tests.

### Course Outcomes (CO's)

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

1. Describe the qualitative analysis by semi micro-qualitative analysis method.
2. Illustrate the preparation of organic compounds.
3. Explain the basic concept and advantages of semi- micro qualitative analysis.
4. Carryout the systematic separation of organic mixtures.
5. Demonstrate the step wise procedure to predict the functional groups present in the organic mixture.
6. Test the functional groups with their special tests.

### Contents

Analysis of two - component mixtures: Separation and characterization of compounds.

*Note: Each student should analyze a minimum of six organic mixtures.*

Preparations involving one stage comprising of the following process: Nitration, acylation, halogenation, diazotisation, rearrangement, hydrolysis, reduction, alkylation and oxidation and one preparation illustrating the following: Benzoin condensation, Cannizzaro reaction, Perkin reaction, Reimer-Tiemann reaction, Sandmeyer reaction, Fries rearrangement, Skraup synthesis- single stage.

*Note: Each student should do a minimum of six preparations involving single stage.*



## SUGGESTED READINGS

1. Thomas, A. O., (2013). Practical Chemistry. Cannanore: Scientific Book Center.
2. Bansal, R. K, (2008). Laboratory Manual of Organic Chemistry (IV Edition). New Delhi: New Age Publishers.
3. Arun Sethi, (2010). Systematic Lab Experiments in Organic Chemistry. New Delhi: New Age Publisher.
4. Furniss, B. S., Hannaford, A. J., Smith, P. W. G., & Tatchell, A. R., (2004). Vogel's Textbook of Practical Organic Chemistry (V Edition). Singapore: Pearson Education Ltd.

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**21CHP112      ORGANIC CHEMISTRY PRACTICAL-II      Semester- I**  
**(QUANTITATIVE ANALYSIS AND DOUBLE STAGE PREPARATIONS)      4H    2C**

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**Instruction Hours/week: L: 0 T: 0 P: 4    Marks: Internal: 40 External: 60 Total: 100**  
**External Semester Exam: 6 Hrs**

### Course Objectives

This course enables the students to

- Understand the basic principles about quantitative analyses.
- Understand the concepts and systematic procedure for estimation and analysis of oils.
- Apply the systematic procedure for estimation of organic compounds.
- Perform synthesis of organic compounds in two stages.
- Analyze the different methods of extraction of natural products.
- Demonstrate the estimation of active constituents present in natural products.

### Course Outcomes (CO's)

On the completion of this course, students understood the

1. The basic principles about quantitative analyses.
2. Concepts and systematic procedure for organic estimations and analysis.
3. Systematic procedure for estimation of organic compounds.
4. Synthesis of organic compounds in two stages.
5. Different methods of extraction of natural products.
6. Demonstrate the estimation of active constituents present in natural products.

### Contents

#### I. Organic Estimations

1. Estimation of Phenol.
2. Estimation of ethyl methyl ketone.
3. Estimation of glucose.
4. Estimation of nitro compound.
5. Estimation of amino compound.
6. Estimation of methoxy groups.
7. Unsaturation of an organic compound.

#### II. Analysis of oils

1. Iodine value of an oil(Reichert- Meissl value)
2. Saponification value of an oil

3. Acetyl value of an oil.

### **III. Double stage preparations**

1. Anthranilic acid and phthalimides.

### **IV. Extraction from Natural Products** (Extraction and estimation of active constituents)

Only for learning purpose and demo (Not for exam)

- a. Lactose from milk.
- b. Caffeine from tea.
- c. Nicotine from tobacco extract.
- d. Citric acid or ascorbic acid from a tablet or from a natural source.
- e. Curcumin from turmeric.
- f. Lycopene from tomato.

### **SUGGESTED READINGS**

1. Arun Sethi, (2010). Systematic Lab Experiments in Organic Chemistry. New Delhi: New Age Publisher.
2. Bansal, R. K, (2008). Laboratory Manual of Organic Chemistry (IV Edition). New Delhi: New Age Publishers.
3. Furniss, B. S., Hannaford, A. J., Smith, P. W. G., & Tatchell, A. R., (2004). Vogel's Textbook of Practical Organic Chemistry (V Edition). Singapore: Pearson Education Ltd.
4. Mendham, J., Denney, R. C., Barnes, J.D., & Thomas, M. (2002). Vogel's textbook of quantitative Chemical Analysis (VI Edition). Singapore: Pearson Education Ltd.

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<b>21CHP201</b>	<b>ORGANIC CHEMISTRY-II</b>	<b>Semester - II</b>
<b>(REARRANGEMENTS, REACTIONS, PHOTOCHEMISTRY AND PERICYCLIC REACTIONS)</b>		<b>4H 4C</b>

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**Instruction Hours/week: L: 4 T: 0 P: 0 Marks: Internal: 40 External: 60 Total: 100**  
**External Semester Exam: 3 Hrs**

### Course Objectives

This course enables the students to

- Gain a versatile knowledge on rearrangements.
- Examine different organic (radical and concerted) reactions and their applications in synthesis.
- Analyze the principles of conformational analysis and stereochemistry.
- Understand the concepts in organic photochemistry.
- Analyze the various theories in pericyclic reactions.
- Implement this basic concept to design and produce the new organic molecules.

### Course Outcomes (CO's)

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

1. Describe various rearrangements in organic chemistry.
2. Understand different types of organic reactions (radical and concerted).
3. Apply the principle of conformational analysis and stereochemistry.
4. Explain the molecular rearrangements, pericyclic reactions and cycloaddition and sigmatropic reactions.
5. Understand the basic ideas of pericyclic reactions.
6. Design new form of organic compounds using these basic concepts.

### UNIT- I Molecular rearrangements

Intramolecular 1,2 - shifts - Wagner - Meerwein and Pinacol-Pinacolone rearrangements.

Migration to carbonyl carbon- Demjanov Neber and Benzil-benzilic acid rearrangements.

Rearrangements to electron deficient nitrogen and oxygen – Baeyer – Villiger, Dienone - phenol, Favorskii, Fries, Wolff, Benzidine, Hoffmann, Beckmann and Stevens rearrangements.

Non-cyclic rearrangements – Chapman and Wallach rearrangements.

### UNIT - II Conformational analysis and stereochemistry

Stereochemistry of sulphur and nitrogen compounds, stereo-selective and stereo-specific reactions - R/S-notation of optically active carbon compounds. Optical isomerism of biphenyls, allenes and spiranes. Planar chirality - cyclophanes and ansa compounds - geometrical isomerism - E/Z notation-configuration in aldoximes and ketoximes.

Conformation in cyclic system—decalins, perhydrophenanthrene and perhydroanthracene. Conformation and reactivity of cyclohexanes.

### **UNIT - III Radical reactions**

Configuration and generation of short lived free radicals-characteristics of free radical reactions – radical substitution, radical additions and rearrangement of free radicals. Typical reactions such as Sandmeyer, Gomberg, Pechmann, Ullmann, Pschorr and Hunsdiecker reactions.

Oxidation and reductions- mechanisms – aromatisation, oxidation of alcohols and glycols, ozonolysis, Sommelet reaction and selectivity in reduction-metal hydride reduction-reduction of nitro compounds and acyloin condensation.

### **UNIT - IV Organic Photochemistry**

Introductory theory of light absorption- Jablonski diagram-photophysical processes-excimers and exciplexes - energy transfer-geometry of excited states – quantum efficiency - photochemical reaction of ketones- Norrish type-I and type-II reactions. Paterno Buchi reaction- cis and trans isomerisation-Photo-Fries rearrangement-Ene reaction- Di-pi methane rearrangement-Barton reaction-photoreduction of ketones.

### **UNIT - V Pericyclic reactions**

Definition-classification-characteristic features- the electrocyclic reaction-Woodward – Hofmann rules- orbital correlation diagram- the Frontier molecular orbital theory-electrocyclic conversion of 1,3-dienes and 1,3,5-trienes. Cycloaddition – [2+2] addition-Diel's Alder reaction- stereochemistry of Diel's Alder reaction. Sigmatropic reactions – [1,3], [1,5] and [3,3] sigmatropic shifts - Cope and Claisen rearrangements.

### **SUGGESTED READINGS**

1. Smith, M. B. (2015). *March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure* (VII Edition). New Jersey: John Wiley & Sons, Inc., Hoboken.
2. Nasipuri, D. (2014). *Stereochemistry of Organic Compounds: Principles and Applications* (III Edition). New Delhi: New Age International (P) Ltd.
3. Mukherji, S. M., & Singh, S. P. (2014). *Reaction Mechanism in Organic Chemistry* (III Edition). New Delhi: Laxmi Publications Pvt. Ltd.
4. Tewari, N. (2011). *Advanced Organic Reaction Mechanism* (III Edition). Kolkata: Books and Allied (P) Ltd.
5. Sanyal, S. N. (2014). *Reactions, Rearrangements and Reagents* (IV Edition). New Delhi: Bharathi Bhawan (Publishers and Distributors).

6. Ramesh, P. (2005). *Basic Principles of Organic Stereochemistry* (I Edition). Madurai: Meenu Publications.
7. Depuy, C. H., & Chapman, O. L. (1975). *Molecular Reactions and Photochemistry* (II Edition). New Delhi: Prentice-Hall of India Private Limited.
8. Coxon, J. M., & Halton, B. (2011). *Organic Photochemistry* (II Edition). New Delhi: Cambridge University Press.
9. Nicholass, J. T., Scaiano J. C., & Ramamurthy, V. (2010). *Modern Molecular Photochemistry of Organic Molecules* (I Edition). United States: University Science Books.

21CHP202

**INORGANIC CHEMISTRY- II  
(CO-ORDINATION CHEMISTRY)****Semester-II****4H 4C****Instruction Hours/week: L: 4 T:0 P: 0    Marks: Internal: 40 External: 60 Total: 100****External Semester Exam: 3 Hrs****Course Objectives**

This course enables the students to

- Understand the theories of bonding in coordination compounds.
- Analyse the kinetics and mechanisms of reactions of complex compounds.
- Understand the magnetic properties of coordination compounds.
- Gain the knowledge on metal carbonyls and organometallic chemistry.
- Analyze the types of organometallic compounds like alkyl, alkene and cyclopentadienyl compounds.
- Evaluate the reaction mechanisms of co-ordination compounds and their biological application.

**Course Outcomes (CO's)**

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

1. Explain the naming of coordination compounds and to be able to draw the structure based on its name.
2. Determine the magnetic properties using crystal field theory (and in simple terms the colour) of coordination compounds.
3. Summarize the stability of metal complexes by the use of formation constants and to calculate thermodynamic parameters from them.
4. Describe metal carbonyls and organometallic chemistry.
5. Classify the types organometallic compounds like alkyl, alkene and cyclopentadienyl compounds.
6. Predict the mechanisms of co-ordination compounds and their biological application.

**UNIT - I Coordination Chemistry and bonding**

Nomenclature, isomerism and methods of preparation of coordination complexes- types of ligands.

Bonding: Valence bond theory- Crystal field theory – Crystal field effects in tetrahedral, octahedral and square planar symmetries. Crystal field stabilization energy - weak and strong fields- spectrochemical series. Molecular orbital theory: based on group theoretical approach. M.O. diagram of Oh, Td & square planar symmetries involving pi bonding- experimental evidence for the presence of pi bonding. Magnetic behaviour of the transition metal ions in crystal field and molecular orbital theories.

## UNIT - II Electronic spectra of complexes

Term symbols for d configuration. Russell-Sander's coupling, L-S coupling and microstate table- determination of terms for  $p^2$ ,  $d^1, d^2$  and  $d^3$  configurations. Hund's rule in the determination of lowest energy state. Characteristics of d-d transition -- selection rules rules for electronic spectra. Weak and strong field limits. Orgel diagram and Tanabe – Sugano energy level diagrams. Spectrochemical series Jahn-Teller tetrahedral distortion and spin orbit couplings. Nephelauxetic effect -charge transfer spectra. Luminescence spectra.

## UNIT - III Metal carbonyls

Definition of organometallic compound - 18 electron rule - effective atomic number rule classification of organometallic compounds - the metal carbon bond types - ionic bond - sigma covalent bond - electron deficient bond - delocalised bond - dative bond - metal carbonyl complexes - synthesis - structure and reactions of metal carbonyls - the nature of M- CO bonding - binding mode of CO and IR spectra of metal carbonyls - metal carbonyls-metal carbonyl anions - metal carbonyl hydrides - metal carbonyl halides - metal carbonyl clusters - Wades rule and isolobal relationship - metal nitrosyls - dinitrogen complexes - dioxygen complexes.

## UNIT - IV Metal Alkyl, Alkene and Cyclopentadienyl complexes

**Metal Alkyl complexes:** Stability and structure - synthesis by alkylation of metal halides - by oxidative addition - by nucleophilic attack on coordinated ligands - metal alkyl and 18 electron rule - reactivity of metal alkyls - M-C bond cleavage reactions - insertion of CO to M-C bonds - double carbonylation.

**Metal Alkene complexes:** Synthesis of alkene complexes by ligand substitution - by reduction and by metal atom synthesis - bonding of alkenes to transition metals - bonding in diene complexes - reactivity of alkene complexes - ligand substitution - reactions with nucleophiles - olefin hydrogenation - hydrosilation - Wacker process - C-H activation of alkenes.

**Cyclopentadienyl complexes:** Metallocenes - synthesis of metallocenes - bonding in metallocenes - reactions of metallocenes -  $Cp_2Fe/Cp_2Fe^+$  couples in biosensors - bent sandwich complexes - bonding in bent sandwich complexes - metallocene halides and hydrides.

## UNIT - V Reactions of coordination compounds

Substitution reactions in square planar and octahedral complexes - Trans effect - mechanism of redox reactions. Theories of Electron transfer reactions-outer sphere mechanism-Marcus theory, inner sphere mechanism, electron transfer in metalloproteins. Homogeneous catalysis by coordination compounds - hydroformylation - carboxylation of methanol - hydrogenation of unsaturated organic compounds. Biochemical importance:



Cytochromes, Haemoglobin, Myoglobin, Cyanocobalamine, Chlorophyll- structure and functions. Fluxional molecules.

### SUGGESTED READINGS

1. Huheey, J. E., Keitler, E. A., & Keitler, R. L. (2012). *Inorganic Chemistry- Principles of Structure and Reactivity* (IV Edition). Singapore: Pearson Education.
2. Malik. Wahid. U, Tuli. G. D and Madan, R.D. (2009). *Selected Topics in Inorganic Chemistry* New Delhi: S. Chand and Co.
3. Sarn, K. (2005). *Co-ordination Chemistry*.(I<sup>st</sup> Edition) New Delhi: Rajat Publications.
4. Catherine, E. H., & Alan G. S. (2012). *Inorganic Chemistry* (IV Edition). England: Pearson Education Limited, Harlow.
5. Cotton, F. A., Wilkinson, G., & Paul. L. (2007). *Basic Inorganic Chemistry* (III Edition). New York: John Wiley & Sons.
6. Chakraborty, D. K. (2012). *Inorganic Chemistry*. (II Revised Edition) New Delhi: New Age International Publishing Pvt. Ltd.
7. Cotton, F. A., Wilkinson, G., Murillo, C. A., & Bochmann, M. (1999). *Advanced Inorganic Chemistry* (VI Edition). New York: John Wiley & Sons.
8. Drago, R. S. (2012). *Physical Methods in Inorganic Chemistry*. New York: Rein Gold Publishing Corporation.
9. Gary L. Miessler, Paul J. Fischer and Donald A. Tarr, (2013). *Inorganic Chemistry*, Pearson

21CHP203

**PHYSICAL CHEMISTRY- II  
(GROUP THEORY AND CHEMICAL KINETICS)**

Semester-II

4H 4C

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**Instruction Hours/week: L: 4 T: 0 P: 0 Marks: Internal: 40 External: 60 Total: 100  
External Semester Exam: 3 Hrs**

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**Course Objectives**

This course enables the students to

- Knowledge about symmetry element and matrices.
- Apply the concept of group theory.
- Understand the fundamental knowledge of chemical kinetics and to establish a relationship between the rate of reaction and the concentration of the reactants (the rate law, or rate equation).
- Apply the chemical kinetics concept to study the mechanisms.
- Analyze the various types of reactions in solution and its effects.
- Evaluate the kinetic theory of gas and various method in fast reactions.

**Course Outcomes (CO's)**

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

1. Describe symmetry element and matrices.
2. Illustrate the concepts in the group theory.
3. Recall the theories of reaction rates, how reaction rates are measured and represented in rate laws.
4. Examine the applications of chemical kinetics in studying mechanisms.
5. Classify the various types of reactions in solution and its effects.
6. Evaluate the the kinetic theory of gas and various method in fast reactions.

**UNIT- I Symmetry elements and Matrices**

Symmetry elements and symmetry operations - definition of identical and equivalent elements configurations - effect of performing successive operations commutative and non-commutative - inverse operations.

Groups and their basic properties - definition of a group - basic properties of a group- definition of abelian - cyclic- isomorphic, finite, infinite groups and subgroup. Symmetry classification of molecules into point groups-Schoenflies symbol (only-difference between point group and space group).

Matrices- Definition of matrix, square matrix, diagonal matrix, null matrix, unit matrix, row matrix, column matrix, symmetric matrix, skew symmetric matrix and conjugate matrix. Multiplication, commutative and non commutative-determination of inverse of a

matrix, block multiplication of matrices-addition and subtraction of matrices.

Matrix notations for symmetry operations of  $C_{2v}$  and  $C_{3v}$  groups-construction of character tables for  $C_{2v}$  and  $C_{3v}$  point groups.

### **UNIT – II Group theory**

Definition of reducible and irreducible representations - irreducible representations as orthogonal vectors - direct product rule, the great orthogonality theorem and its consequences - determinations of the characters for irreducible representation of  $C_{2v}$  and  $C_{3v}$  point groups using the orthogonality theorem.

Group theory and Vibrational spectroscopy - vibrational modes as basis for group representation - symmetry selection rules for IR and Raman spectra, Mutual exclusion principle - classification of vibrational modes.

### **UNIT - III Chemical Kinetics**

Rates of chemical reactions, kinetics of first, second and third order reactions and complex methods of determining rate laws, order and molecularity concepts.

**Theories of reaction rates:** Arrhenius theory- hard - sphere collision theory of gas – phase reactions. Potential energy-surfaces, Activated complex theory or Absolute reaction rate theory (ARRT) for ideal gas reactions (formation in terms of partition functions). Relation between activated complex theory and hardsphere collision theory. Thermodynamic formulation-activated complex theory (Enthalpies and entropies of activation)

### **UNIT - IV Reactions in solution**

Comparison between gas-phase and solution reactions. The influence of the solvent on the reactions between ions, reactions between ions and neutral molecules. Influence of ionic strength on rates of reactions in solution - primary salt effect-influence of pressure on rate of reactions in solution -significance of volume and entropy of activation. Secondary salt effect.

Parallel reactions of the same order (first and second, parallel first and second order reactions). Reversible reaction of the same order (first or second order). First order forward and second order backward. Consecutive first order reactions, steady state and rate determining step (or equilibrium) approximation of complex reactions. Chain reactions and explosions.

### **UNIT-V Fast reactions**

Study of fast reactions by Flow methods, pulse methods, relaxation methods, shock-tube method and nuclear magnetic resonance method.

## **Kinetic theory of gases**

Postulates-Maxwell distribution of molecular velocities-Expressions for most probable velocity, average velocity, root mean square velocity. Collision diameter, collision frequency, Mean free path. Transport properties of gases-thermal conductivity, viscosity, diffusion-principle of equipartition of energy.

## **SUGGESTED READINGS**

1. Raman, K.V. (2002). Group Theory and its Applications to Chemistry. New Delhi: Tata McGraw Publishing Company.
2. Cotton, F. A. (2003). Chemical Applications of Group Theory (III Edition). Texas: A Wiley Inter Science Publication.
3. Veera Reddy, K. (2009). Symmetry and Spectroscopy of Molecules. New Delhi: New Age International Pvt. Ltd.
4. Bahl, A., Bahl, B. S., & Tuli, G. D, (2014). Essentials of Physical Chemistry (VEdition). New Delhi: S. Chand & Company.
5. Puri, B.R., Sharma, L.R., & Pathania, M.S. (2015). Elements of Physical Chemistry. Jalandhar: Vishal Publishing House.
6. Laidler, K. J. (2004). Chemical Kinetics (III Edition). New Delhi: Pearson Education Publishing. Indian Branch.
7. Gurdeep Raj, Chemical Kinetics, Goel Publishing House.
8. A.A.Frost and R.G.Pearson, Kinetics and Mechanism, Wiley Eastern, Pvt. Ltd.

**Course Objectives**

This course enables the students to

- Understand the fundamentals of instrumentation techniques.
- Calibrate instruments and validation of analytical methods.
- Gain knowledge on the separation techniques.
- Evaluate the basic instrumental setup, working and its applications.
- Analyze the electro analytical techniques and its applications.
- Understand the principles of volumetric analysis and its calculations.

**Course Outcomes (CO's)**

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

1. Explain the fundamentals of instrumentation techniques.
2. Calibrate instruments and validation of analytical methods.
3. Describe the separation techniques.
4. Justify the basic instrumental setup, working and its applications.
5. Elaborate the electro analytical techniques and its applications.
6. Do volumetric analysis and its calculations.

**UNIT-I Errors in chemical analyses**

Accuracy and propagation of errors, Statistical data analysis and evaluation: Confidence intervals, statistical aids to hypothesis testing- analysis of variance and Regression analysis.

**UNIT-II Calibration of instruments and validation of analytical methods**

**Calibration:** Burette Calibration, Pipette Calibration, Thermometer calibration, UV Spectrophotometer – Absorption and wavelength calibration, HPLC – flow rate calibration, Absorption and wavelength calibration, Theoretical plate calculation etc.

**Analytical method validation:** Linearity and Range, Accuracy, Precision, Specificity, Limit of detection, Limit of Quantitation, Ruggedness and Robustness – Explanation specific to minimum 3 examples.

**UNIT-III Separation techniques**

Solvent extraction - Methods of extraction and applications of solvent extraction. Chromatography- thin layer chromatography, ion exchange chromatography and size exclusion chromatography–HPLC-outline study of instrument modules. Gas chromatography – basic instrumental set up-carriers, columns, detectors and comparative study of TCD, FID, ECD and NPD. Theory & applications –electrophoresis- theory and applications.

#### **UNIT-IV Electroanalytical techniques**

Potentiometry - electrode systems, direct potentiometric titrations-null-point potentiometry and applications. polarography, stripping voltammetry & Amperometric techniques-diffusion currents, Half-wave potentials, construction & characteristics of the DME-quantitative analysis-amperometric titrations and applications of polarography-electrogravimetry and coulometry - coulometry at constant potential, coulometric titrations-conductometric titrations.

#### **UNIT-V Volumetric Analysis**

Types of titrations: Acid base, complexometric, precipitation, and redox titrations.

Theories of Indicators: Common indicators used in acid base, complexometric, precipitation and redox titrations.

Concentration: Molarity, Molality, Normality, including exercises on how to prepare different concentrations of various solutes.

Standardisation of volumetric solutions, using primary standards. Calculations in volumetric Analysis

#### **SUGGESTED READINGS**

1. Geeffery, G.H., (1989). *Vogel's Text Book of Quantitative Chemical Analysis*, ELBS Edn.
2. Skoog, A.K., West, D.M., Holler, F.J., & Crouch, S.R. (2004). *Fundamentals of Analytical Chemistry*, 8th edition, Thomson Brooks Cole.
3. Rouessac, F. and Rouessac, A. (). *Chemical Analysis: Modern Instrumentation Methods and Techniques*, 2ndEdn, John Wiley and Sons.
4. Skoog, A., Holler, E.J., & Crouch, S.R. (2007). *Principles of Instrumental Analysis*, 6th edition, Thomson Brooks Cole.
5. Fifield, F.W. and Kealey, D. (1983). *Principles and Practice of Analytical Chemistry*, 2nd Edition, International Book Company, London.
6. Willard, H.H., Merrit, L.L., Dean, J.A., and Settle, F.A. (1986). *Instrumental Methods of Analysis*. CBS Publishers, New Delhi.

21CHP205A

CATALYSIS

Semester - II

4H 4C

**Instruction Hours/week: L: 4 T: 0 P: 0 Marks: Internal:40 External: 60 Total:100**  
**External Semester Exam: 3 Hrs**

**Course Objectives**

This course enables the students to

- Understand the fundamentals of catalysis.
- Analyze the role of homogenous catalyst in various organic synthesis.
- Apply the characterization techniques to solid catalysts.
- Evaluate the property of heterogeneous catalyst and its application among various chemical reactions & synthesis.
- Analyze the photocatalyst and its environmental applications.
- Differentiate homogenous, heterogeneous and photo catalysis.

**Course Outcomes (CO's)**

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

1. Explain the fundamentals of catalysis and characterization techniques.
2. Analyze the homogenous catalysis in various organic syntheses.
3. Illustrate the characterization techniques for solid catalysts.
4. Evaluate the property of heterogeneous catalysis and its application among various chemical reaction & synthesis.
5. Examine the photo catalysis and its environmental applications.
6. Differentiate homogenous, heterogeneous and photo catalysis.

**Unit - I Fundamentals of catalyst**

Fundamentals: Catalyst-activation energy concept-types of catalysis-comparison of homogeneous & heterogeneous catalysis - enzyme catalysis - green catalysis- nano catalysis- autocatalysis - phase transfer catalysis - promoters - poisons - examples.

**Unit - II Homogeneous catalysis**

Homogeneous catalysis: Noyori asymmetric hydrogenation -metal mediated C-C and C-X coupling reactions - Heck, Stille, Suzuki, Negishi and Sonogashira, Nozaki-Hiyama, Buchwald-Hartwig- directed orthometalation - metal (Rh, Ir) catalyzed C-H activation reactions and their synthetic utility -copper and rhodium based carbene and nitrene complexes - cyclopropanation - Rh catalyzed C-H insertion and aziridination reactions including asymmetric version -introduction to N-heterocyclic carbene metal complexes.

**Unit - III Characterization of Solid catalysts**

Characterization of solid catalysts: Surface area - structure - surface morphology - porosity -pore volume - diameter - particle size - X-ray diffraction - SEM, TEM, X-ray absorption

spectroscopy, XPS and Auger spectroscopy to surface studies - TPD, TPR for acidity and basicity of the catalysts - theories - boundary layer theory -Volkenstein theory - Balanding's approach.

#### **Unit - IV Heterogeneous catalysis**

Heterogeneous catalysis: Adsorption isotherms - surface area - pore size and acid strength measurements -porous solids -catalysis by metals - semiconductors and solid acids – supported metal catalysts -catalyst preparation - deactivation and regeneration -model catalysts -ammonia synthesis -hydrogenation of carbon monoxide -hydrocarbon conversion–selective catalytic reduction - polymerization.

#### **Unit - V Photo catalysis**

Photo catalysis: Porphyrins -phthalocyanines and semiconductor as photo catalysts in photolysis reactions - generation of hydrogen by photo catalysts - photocatalytic break down of water and harnessing solar energy - photocatalytic degradation of dyes – environmental applications.

#### **SUGGESTED READINGS**

1. Emmet, P. H. (1954). Catalysis (Vol I and II). Reinhold.
2. Schlosser, M. (1996). Organometallics in Synthesis, A Manual. John Wiley.
3. Hegedus, L.S. (1999). Transition Metals in the Synthesis of Complex Organic Molecules. University Science.
4. Chakrabarty, D. K & and B. Viswanathan, B. (2008). Heterogeneous Catalysis, New Age.
5. Viswanathan, B., Kannan, B. & R.C. Deka, (2010). Catalysts and Surfaces: Characterization Techniques. Narosa.
6. Kaneko M. & Okura, I. (2003). Photo catalysis: Science and Technology. Springer.



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		<b>Semester - II</b>
<b>21CHP205B</b>	<b>INDUSTRIAL ORGANIC SYNTHESIS</b>	<b>4H 4C</b>

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**Instruction Hours/week: L: 4 T: 0 P: 0 Marks: Internal: 40 External: 60 Total: 100**  
**External Semester Exam: 3 Hrs**

**Course Objectives**

This course enables the students to

- Remember the concept of retrosynthesis and the terms involved.
- Understand the one group and two group disconnections.
- Illustrate the methods for protection and deprotection of important functional groups.
- Evaluate the use of important reagents in organic synthesis.
- Design reagents for selected name reactions in Organic synthesis.
- Develop a method for organic synthesis in industries.

**Course Outcomes (CO's)**

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

1. Spell out the concept of retrosynthesis and the terms involved.
2. State the one group and two group disconnections.
3. Discuss the various protection and deprotection of important functional groups.
4. Use important reagents in organic synthesis.
5. Investigate the selected name reactions in organic synthesis.
6. Develop a method for organic synthesis in industries

**UNIT - I Introduction to retrosynthesis**

Synthon, synthetic equivalent, target molecule, functional group interconversion, disconnection approach, importance of the order of events in organic synthesis. Chemoselectivity, one group C-C and C-X disconnection (disconnection of alcohols, alkenes, and carbonyl compounds).

**UNIT - II Two group C-C & C-X disconnections**

1,3 and 1,5 Difunctionalised compounds,  $\alpha,\beta$ - unsaturated carbonyl compounds, control in carbonyl condensation, synthesis of 3,4,5 and 6 membered rings in organic synthesis. Diels- Alder reaction, Connection in retro synthesis.

**UNIT - III Protecting groups**

Protection of hydroxyl, carboxyl, carbonyl, amino groups. Umpolung reagents, definition of umpolung, acyl anion equivalent, Protection of carbon-carbon multiple bonds. Illustration of protection and deprotection in synthesis.

## **UNIT - IV Organic Reagents**

Use of the following reagents in organic synthesis and functional group transformation, 1,3-Dithianes, *N*-Bromosuccinimide, Organolithium reagents, Sodamide, Organosilicon compounds, Diazomethane, Periodic acids, Pyridinium chlorochromate (Corey's reagent), Lead tetraacetate, Fenton's reagent, Phase transfer catalyst, Crown ethers, Merrifield resin, Wilkinson's catalyst and Baker yeast.

## **UNIT - V Name reactions in organic synthesis**

Peterson olefination, McMurry, Shapiro reaction, Bomford-Stevens reaction, Palladium based reactions- Suzuki, Heck, Sonogashira, Hiyama, Stille, Glaser-Eglinton coupling, Henry reaction, Birch reduction, Clemmensen reduction, Dess-Martin oxidation, Hofmann-Löffler-Freytag reaction, Etard reaction, Baylis Hillman reaction, Wolff- Kishner reduction.

## **SUGGESTED READINGS**

1. Warren,S. (2010). Organic Synthesis the Disconnection approach, Wiley and sons,
2. Renuga,S. (2016). Name reactions and reagents in organic synthesis, Vishal Publishing Co. Jalandhar-Delhi.
3. Nasir Hussain and Saba Khan, (2016). Reactions and Reagents, Himanshu Publications, New Delhi.
4. Clayden, J., Greeves, N. & Warren, S. (2012). Organic Chemistry (II Edition). Oxford University Press, Oxford.
5. Sanyal, S. N. (2014). Reactions, Rearrangements and Reagents (IV Edition). New Delhi: Bharathi Bhawan (Publishers and Distributors).
6. Smith, M. B. (2015). March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure(VII Edition). New Jersey: John Wiley & Sons, Inc., Hoboken.

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<b>21CHP205C</b>	<b>ADVANCED ENERGY STORAGE</b>	<b>Semester - II</b>
		<b>4H 4C</b>

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**Instruction Hours/week: L: 4 T: 0 P: 0 Marks: Internal: 40 External: 60 Total: 100**  
**External Semester Exam: 3 Hrs**

### Course Objectives

This course enables the students to

- Understand the efficiency of a battery by charge/discharge cycle.
- Differentiate hydrogen fuel cells and other types of fuel cells and other energy storage devices.
- Understand the energy and charge added during the battery charge/discharge cycle.
- Identify the other energy storage devices such as ultra-capacitors, flywheels, and compressed air.
- Analyze the technology behind battery electric and hybrid vehicles.
- Evaluate the effects of burning fossil fuels on air quality and climate change.

### Course Outcomes (CO's)

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

1. Define the energy efficiency and Columbic efficiency for a battery charge/discharge cycle.
2. Compare the operation of batteries to hydrogen fuel cells and other types of fuel cells, including infrastructure needs.
3. Measure the energy added and charge added during charging or discharging of a battery and calculate the C-rate for battery charging.
4. Identify other energy storage devices such as ultra-capacitors, flywheels, compressed air.
5. Compare different batteries used in recent battery electric and hybrid vehicles.
6. Evaluate the effects of burning fossil fuels on air quality and climate change.

### UNIT - I Electrochemistry

Conductance- Transport number - Debye-Huckel-Onsager equation - Falkenhagen effect, Wein effect - ionic strength, Debye-Huckel limiting law and its verifications - electrode potential - concentration cells - liquid junction potential

Electrokinetic phenomena- theories of double layer – Helmholtz-perrin, Guoy Chapmann & Stern theories - Theories of over voltage and zeta potential - electrodictics - mechanism of electrode reactions - polarization and over potential - Butler Volmer equation - electrophoresis and electro osmosis.

## **UNIT - II Electrochemistry**

The reaction quotient,  $Q$ , for a chemical reaction - The potential,  $E$ , for non-standard conditions using the Nernst Equation - Rates of reactions and types of over-voltages in galvanic and electrolytic cells and the Tafel Equation - Efficiency of chemical energy conversion: batteries versus heat engines.

## **UNIT - III Introduction to Batteries**

Primary cells - Secondary batteries - Battery charging and discharging curves for secondary batteries - Specific power and specific energy, Ragone plot - Energy efficiency of batteries, energy out during discharge  $\div$  energy in during charge - Energy efficiency of batteries versus that of heat engines for converting chemical energy into work

## **UNIT - IV Batteries for Electric and Hybrid Vehicles**

Battery packs, voltage and state of charge, coulomb counting - Energy in a battery (kW h) and charge in a battery (A h); C-rate of charging and discharging, Peukert Equation - Coulombic efficiency of batteries and battery lifetime - Battery pack control module.

## **UNIT - V Additional Energy Storage Devices and Renewable Energy**

Hydrogen and Fuel Cells: Types of fuel cells - Construction and operation of fuel cells- Proton exchange membrane (PEM) fuel cells using hydrogen for powering vehicles. Hydrogen fueling system and hydrogen storage aboard vehicles- Comparison of fuel cells and batteries for powering electric vehicles. Capacitors: storing charge- Flywheels: storing kinetic energy - Compressed air: storing potential energy - Renewable energy and synergy with electric vehicles.

## **SUGGESTED READINGS:**

1. Aubrecht, G. (2005). Energy: Physical, Environmental, and Social Impact (III Edition). San Francisco, CA: Pearson Addison-Wesley.
2. Giancoli, D. G. (2014). Physics: Principles with Applications (VII Edition). Upper Saddle River, NJ: Prentice Hall.
3. McMurry, J. E. & Fay, R. C. (2012). Chemistry (VI Edition). Upper Saddle River, NJ: Prentice Hall.

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21CHP211	INORGANIC CHEMISTRY PRACTICAL-I (QUALITATIVE ANALYSIS AND PREPARATIONS)	Semester - II 4H 2C
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Instruction Hours/week:L: 0 T: 0 P: 4 Marks: Internal: 40 External: 60 Total:100  
External Semester Exam: 6 Hrs

### Course Objectives

This course enables the students to

- Understand the qualitative analysis by semi micro-qualitative analysis method.
- Prepare inorganic complexes.
- Describe the basic concept and advantages of semi- micro qualitative analysis.
- Understand the systematic separation d-block elements.
- Apply the step wise procedure to predict the anions along with metals.
- Analyze the d-block elements with their special tests.

### Course Outcomes (CO's)

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

1. Understand the qualitative analysis by semi micro-qualitative analysis method.
2. Prepare inorganic complexes.
3. Describe the basic concept and advantages of semi- micro qualitative analysis.
4. Understand the systematic separation d-block elements.
5. Experiment the anions and cations of the metals by using step wise procedure.
6. Analyze the d-block elements with their special tests.

### Contents

Thallium, Tungsten, Selenium, Tellurium, Molybdenum, Cerium, Thorium, Titanium, Zirconium, Vanadium, Beryllium, Uranium and Lithium.

*Note: Each student should analyze a minimum of six inorganic mixtures.*

### About ten preparations involving different techniques selected from the following:

Lead tetra acetate, dipyrindinium hexaplumbate, hydroxylamine hydrochloride, ortho and para- hydroxy phenyl mercuric chloride, potassium cupric chloride, chrome alum, copperI chloride, tris(thio urea) copper(I) Chloride, potassium trioxalato- aluminato(III), potassium trioxalato-chromate(III), potassium trioxalato- ferrate(III), hexammine cobalt(III)chloride, chloropentammine chromium(III), chloro aquo pentammine chromium(III) nitrate, tetrammine copper(II) sulphate, ammonium hexa chloro stanate(IV).

*Note: Each student should do a minimum of ten preparations.*

## SUGGESTED READINGS

1. Ramanujam, V. V. (2004). *Inorganic Semi-micro Qualitative Analysis* (III Edition). Chennai: The National Publishing Company.
2. Venkateswaran, V., Veeraswamy, R., & Kulandaivelu, A. R. (2004). *Basic Principles of Practical Chemistry* (II Edition). New Delhi: S. Chand Publications.
3. Siddhiqui, Z. N. (2002). *Practical Industrial Chemistry* (I Edition). New Delhi: Anmol Publications Pvt. Ltd.
4. Mendham, J. R., Denney, C., Barnes, J. D., & Thomas, M. (2002). *Vogel's Textbook of Quantitative Chemical Analysis* (VI Edition). Singapore: Pearson Education Ltd.
5. Lepse, P. A., & Peter, L. B. (1986). *Lab Manual for Lingren's Essentials of Chemistry*. New Delhi: Prentice Hall.
6. Srivastava.T.N., & Kamboj. P.C., *University Practical Chemistry* (2013). New Delhi. Milestone Publishers and Distributors.

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**Semester - II**

**21CHP212          INORGANIC CHEMISTRY PRACTICAL - II          4H   2C**  
**(QUANTITATIVE ANALYSIS AND COMPLEX PREPARATIONS)**

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**Instruction Hours/week: L: 0 T: 0 P: 4 Marks: Internal: 40 External: 60 Total: 100**

**External Semester Exam: 6 Hrs**

### **Course Objectives**

This course enables the students to

- Remember the basic principles about quantitative analyses.
- Understand the concepts and systematic procedure in gravimetric analysis.
- Apply the systematic procedure for estimation.
- Apply the synthetic method to prepare in-organic co-ordination complexes.
- Analyze the molecules and identify its nature through chromatography technique.
- Apply this ideas and concepts to water treatment process, food science and forensic fields.

### **Course Outcomes (CO's)**

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

1. Remember the basic principles about quantitative analyses.
2. Explain the concepts and systematic procedure in gravimetric analysis.
3. Apply the systematic procedure for estimation.
4. Synthesise in-organic co-ordination complexes
5. Separate and identify compounds through chromatography technique.
6. Illustrate concepts to water treatment process, food science and forensic fields.

### **Contents**

#### **I. Analysis of mixture of ions - volumetry and gravimetry**

1. Estimation of copper and nickel
2. Estimation of calcium and barium
3. Estimation of nickel and zinc

#### **II. Titrimetry**

1. Oxidation using ceric salts.
2. Oxidation using vanadium salts.

#### **III. Chromatography**

1. Column chromatography
2. Paper chromatography
3. Thin layer chromatography

#### **IV. Colorimetric analysis**

**Estimation of copper, nickel, zinc, lead, chromium, Iron**

#### **V. Analysis of cement**

#### **VI. Titrations in non aqueous solvents.**

#### **VII. Preparation, analysis and study of co-ordination complexes (any 5).**

### **SUGGESTED READINGS**

1. Lapse, P. A., & Peter, L. B. (1986). *Lab Manual for Lingren's Essentials of Chemistry*. New Delhi: Prentice Hall.
2. Mendham, J. R., Denney, C., Barnes, J. D., & Thomas, M. (2002). *Vogel's Textbook of Quantitative Chemical Analysis* (VI Edition). Singapore: Pearson Education Ltd.
3. Ramanujam, V. V. (2004). *Inorganic Semi-micro Qualitative Analysis* (III Edition). Chennai: The National Publishing Company.
4. Siddhiqui, Z. N. (2002). *Practical Industrial Chemistry* (I Edition). New Delhi: Anmol Publications Pvt. Ltd.
5. Venkateswaran, V., Veeraswamy, R., & Kulandaivelu, A. R. (2004). *Basic Principles of Practical Chemistry* (II Edition). New Delhi: S. Chand Publications.
6. Srivastava.T.N., & Kamboj. P.C., *University Practical Chemistry* (2013). New Delhi. Milestone Publishers and Distributors.



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21CHP301	<b>ORGANIC CHEMISTRY- III (NATURAL PRODUCTS)</b>	<b>Semester-III 4H 4C</b>
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**Instruction Hours/week: L: 4 T: 0 P: 0 Marks: Internal: 40 External: 60 Total: 100  
External Semester Exam: 3 Hrs**

**Course Objectives**

This course enables the students to

- Understand the importance of natural products.
- Classify the terpenoids and its application.
- Determine the structure of steroids and do its synthesis.
- Evaluate the importance of alkaloids in medicinal field and its synthesis.
- Analyze the various proteins and enzymes.
- Understand the significance of nucleic acids.

**Course Outcomes (CO's)**

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

1. Understand the importance of natural products.
2. Classify the terpenoids and its applications.
3. Determine the structure of steroids and do its synthesis.
4. Evaluate the importance of alkaloids in medicinal field and its synthesis.
5. Analyse the proteins and enzymes.
6. Illustrate the importance of nucleic acids.

**UNIT - I**

**Terpenoids:** Introduction-General properties of terpenoids- Isolation-Isoprene rule-Gem-dialkyl rule-Classification of terpenoids-general methods of determining structure of terpenoids –structural elucidation and synthesis of Zingiberene, Eudesmol, Abietic acid, Caryophyllene and Santonin-biosynthesis of monoterpenoids.

**UNIT - II**

**Steroids:** Introduction – structural elucidation and synthesis of Cholesterol (synthesis not necessary), Ergosterol, Vitamin D, Equilenin, Oestrone, Testosterone and Progesterone. Bile acids – biosynthesis of sterols.

**UNIT-III**

**Alkaloids:** Definition of an alkaloid-extraction of alkaloids-general properties - general methods of determining structure of alkaloids – structural elucidation and synthesis of Atropine, Morphine and Quinine -biosynthesis of quinoline alkaloids.

## UNIT-IV

**Proteins:** General nature of proteins - classification of proteins –the peptide linkage-the primary structure of peptides- synthesis of peptides– oxytocin-insulin. The spatial arrangements of protein molecules-introduction-secondary, tertiary, and structure of proteins-quaternary structure of proteins.

**Enzymes:** General nature of enzymes-nomenclature and classification-cofactors–specificity of enzyme action- mechanism of enzyme action.

## UNIT- V

**Nucleic acids:** Introduction-classification of nucleic acids-relation among nucleic acids, nucleotides and nucleosides-isolation of nucleic acids-components of nucleic acids-constitution of nucleic acids-structure of nucleosides- structure of nucleotides-sequence of nucleic acids-structure of DNA- structure of RNA.

### SUGGESTED READINGS:

1. Chatwal, G. R. (2015). *Organic Chemistry of Natural Products Vol. II*. New Delhi: Himalaya Publishing House.
2. Finar, I. L. (2013). *Organic Chemistry Vol. II: Stereochemistry and the Chemistry of Natural Products* (V Edition). New Delhi: Pearson Education, Ltd.
3. Chatwal, G. R. (2015). *Organic Chemistry of Natural Products. Vol. I*. New Delhi: Himalaya Publishing House.
4. Saluja, M. P., Raj Kumar & Anuja Agarwal (2017). *Advanced Natural Products* (Revised IV Edition). Meerut: Krishna Prakashan Media (P) Ltd.

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21CHP302	<b>PHYSICAL CHEMISTRY- III (THERMODYNAMICS)</b>	<b>Semester-III 4H 4C</b>
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**Instruction Hours/week: L: 4 T:0 P:0    Marks: Internal:40 External: 60 Total:100  
External Semester Exam: 3 Hours**

### Course Objectives

This course enables the students to

- Understand thermodynamics and non-ideal systems.
- State and explain the third law of thermodynamics.
- Analyse the classical Maxwell-Boltzmann and quantum statistics.
- Know about partition functions and determining thermodynamic properties.
- Understand the importance of heat capacity of solids.
- Apply the thermodynamic factors to various organic synthesis processes (how the reaction condition and reaction rate various depend on the thermodynamic factors).

### Course Outcomes (CO's)

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

1. Understand thermodynamics and non-ideal systems.
2. Describe the third law of thermodynamics.
3. Analyse the classical Maxwell-Boltzmann and quantum statistics.
4. Explain about partition functions and determining thermodynamic properties.
5. Understood heat capacity of solids.
6. Apply the thermodynamic factors to various organic synthesis processes (how the reaction condition and reaction rate various depend on the thermodynamic factors).

### UNIT - I

**Thermodynamics and Non-ideal systems:** Chemical potential and the definition of fugacity. Determination of fugacity of gases by graphical method and from equations of state. Variation of fugacity with temperature. Fugacity and the standard states for non ideal gases.

Definition of activity. Activity coefficient. Temperature coefficient of activity. Standard states. Applications of activity concept to solutions. The rational and practical approaches. Measurement of activity of solvent from colligative properties. Determination of activity of solute.

## UNIT - II

**Third Law of Thermodynamics:** Probability and third law. Need for third law. Nernst heat theorem and other forms stating third law. Thermodynamic quantities at absolute zero. Statistical meaning of third law and apparent exception. Entropy changes in chemical reactions, entropies of real gases, residual entropy.

Mathematical Introduction: Theories of permutation & combination, laws of probability.

Distribution laws. Gaussian distribution.

## UNIT - III

**Classical Maxwell – Boltzmann Statistics:** Maxwell distribution law for molecular velocities and molecular speeds in an ideal gas. Velocity and speed distribution functions. Experimental verification of Maxwell distribution law. Evaluation of average speed, root mean square speed and most probable speed from distribution law. Distribution function in terms of the kinetic energy of an ideal gas. The principle of equipartition of energy and the calculation of heat capacities of ideal gases. Limitations of the principle of equipartition of energy.

**Quantum statistics:** Maxwell-Boltzmann statistics. Thermodynamic probability. Thermodynamic probabilities of systems in equilibrium. Boltzmann expression for entropy. Stirling's approximation. State of maximum thermodynamics probability. Lagrangian multipliers. Thermodynamic probabilities of systems involving energy levels. Maxwell-Boltzmann distribution law. Evaluation of alpha and beta in MB distribution law.

## UNIT - IV

**Partition function:** Definition, justification of nomenclature, microcanonical and canonical ensembles. Molecular partition and canonical function. The relation between the total partition function of a molecule and the separate partition functions. Translational partition function, rotational partition function. Effect of molecular symmetry on rotational partition function. Ortho and para hydrogen. Vibrational partition function. Electronic partition function. Evaluation of thermodynamic properties  $E$ ,  $H$ ,  $S$ ,  $A$ ,  $G$ ,  $C_v$  and  $C_p$  from monoatomic and diatomic ideal gas molecules partition functions. Thermodynamic properties of polyatomic ideal gases. Calculation of equilibrium constants of reaction involving ideal gases from partition functions.

## UNIT - V

**Heat capacities of solids:** Einstein's and Debye's theories of heat capacities of solids. Bose-Einstein and Fermi-Dirac Statistics: Bose Einstein distribution law- Entropy of Bose Einstein gas. Planck distribution law of black body radiation. Fermi-Dirac

distribution law. Entropy of a Fermi-Dirac gas. Heat capacities of the electron gas and the heat capacities of metals. Negative absolute temperature.

**SUGGESTED READINGS:**

1. Glasstone, S. (2008). *Thermodynamics for Chemists*. New York: Litton Edition Publishing.
2. Atkins, P., & De Paula, J. (2014). *Atkins Physical Chemistry* (X Edition). Oxford: Oxford University Press.
3. Kapoor, K. L. (2015). *Text Book Physical Chemistry Vol. V*. New Delhi: MacMillan India Ltd.
4. Lavin, I. N. (2002). *Physical Chemistry* (V Edition). New Delhi: Tata-McGraw Hill Publishing Company.
5. Whittakar, A. G. (2001). *Physical Chemistry*. New Delhi: Mount & Heal Viva Books Pvt. Ltd.
6. Puri, B.R., Sharma, L.R., & Pathania, M.S. (2013) . *The Principles of Physical Chemistry*. Vishal Publishing Co.,

21CHP303	<b>PHYSICAL METHODS IN CHEMISTRY (INSTRUMENTATION)</b>	<b>Semester -III 4H 4C</b>
<b>Instruction Hours/week: L:4 T:0 P:0 Marks: Internal:40 External: 60 Total:100 External Semester Exam: 3 Hours</b>		

**Course Objectives**

This course enables the students to

- Understand the working of an electron microscope.
- Analyse samples through electron spectroscopy and various methods in thermal analysis.
- Perform circular dichroism and optical rotatory dispersion.
- Explain the electron spin resonance spectroscopy.
- Know about flame emission spectroscopy.
- Apply the chromatographic and spectroscopic concepts for separation and identification of mixture compounds/complex/metals.

**Course Outcomes (CO's)**

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

1. Understand the working of various electron microscope.
2. Analyse samples through electron spectroscopy and thermal analysis.
3. Perform circular dichroism and optical rotatory dispersion.
4. Describe the Electron Spin Resonance spectroscopy.
5. Know about flame emission spectroscopy.
6. Apply the chromatographic and spectroscopic concepts for separation and identification of mixture compounds/complex/metals.

**UNIT – I Microscopic techniques**

Scanning and Transmission Electron Microscopy, Scanning Probe Microscopies:- Atomic Force, scanning tunneling microscopy, Diffraction and scattering techniques, Vibrational spectroscopy, Surface techniques.

**UNIT– II Thermal analysis and Electron spectroscopy**

**Thermal analysis:** Differential thermal analysis DTA and differential scanning calorimetry DSC - basic principles - thermo gravimetric analysis. Thermo mechanical analysis (TMA) and Dynamic mechanical analysis (DMA)-Instrumentation and applications

**Electron spectroscopy:** ESCA XPS: Principle, chemical shifts - description of ESCA spectrometer, X-ray sources, samples, analysis, detectors and recording devices-applications.

Auger electron spectroscopy AES and Ultra-Violet photo electron spectroscopy UPS/PES principles and applications.

### **UNIT– III Diffraction methods and Raman spectroscopy**

**Diffraction Methods:** Single crystal and Powder X–Ray Diffraction and their applications for Inorganic Compounds, Neutron Diffraction and Electron Diffraction.

**Raman spectroscopy:** Stokes and anti-Stokes lines. Polarizability ellipsoids. Rotational and vibrational. Selection rules. Rule of Mutual Exclusion. Polarization of Raman lines.

### **UNIT – IV ESR spectroscopy**

Theory - derivative curves - g shift - hyperfine splitting-isotropic and anisotropic systems-zero field splitting and Kramer degeneracy. Identification of free radicals – applications to copper complexes.

### **UNIT – V Atomic spectrometry**

Atomic absorption spectroscopy (AAS): Absorption of characteristic radiation, instrumentation, Hollow cathode lamp – sampling- quantitative measurements and interferences – atomic emission- instrumentation, plasma sources – instrumentation – inductively coupled plasma–mass spectrometry (ICP-MS) – principles & Instrumentation and applications of flame emission spectrometry – flame characteristics & processes – applications of flame photometry and flame atomic emission spectrometry.

### **SUGGESTED READINGS:**

1. Gopalan, V., Subramanian, P. S., & Rangarajan, K. (2003). *Elements of Analytical Chemistry*. New Delhi: S. Chand and Sons.
2. Usharani, S. (2002). *Analytical Chemistry*. Chennai: MacMillan India Ltd.
3. Sharma, B. K. (2019). *Instrumental Methods of Chemical Analysis* (27<sup>th</sup> Edition). Meerut: Krishna Prakashan Media (P) Ltd.
4. Ewing, G. W. (1988). *Instrumental Methods of Chemical Analysis* (III Edition). Singapore: McGraw Hill International Edition.
5. Gurdeep. R. Chatwal, & Sham K Anand. (2018). *Instrumental Methods of Chemical Analysis* (V Edition). New Delhi: Himalaya Publishing House.
6. Drago, R .S. (2012). *Physical Methods in Inorganic Chemistry*. New York: Reinhold Publishing Corporation.
7. Skoog, D. A., & West, D. M. (2004). *Fundamentals of Analytical Chemistry* (VIII Edition). Singapore: Thomson Book Store.
8. Svehla, G. (2002). *Vogel's Qualitative Inorganic Analysis* (VII Edition). Singapore. Pearson Education

21CHP304

NANOCHEMISTRY

Semester-III

4H 4C

**Instruction Hours/week: L: 4 T: 0 P: 0 Marks: Internal: 40 External: 60 Total: 100**  
**External Semester Exam: 3 Hours**

### Course Objectives

This course enables the students to

- Understand the history and perspectives of nanotechnology.
- Analyze the various types of 1D, 2D and 3D nanoparticles.
- Analyze the various types of carbon nanotubes and its application.
- Understand carbon based nanomaterials and its properties.
- Apply the theoretical concepts to study the properties of nano materials.
- Motivate and lead the student in the field of nanotechnology.

### Course Outcomes (CO's)

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

1. Understand the history and perspectives of nanotechnology.
2. Analyse various types and significant of 1D, 2D and 3D nanoparticles.
3. Compare the various types of carbon nanotubes and its application.
4. Discuss about carbon based nanomaterials and its properties.
5. Illustrate the theoretical concepts to study the properties of nano materials.
6. Motivate and lead them in the pathway of nanotechnology.

### UNIT - I Fundamentals- Size & Scale Units

Definitions and course organization, Historical development of nanomaterials, Classification of nanomaterials.

Scaling Atoms, Molecules, Clusters and Supramolecules. Structure and Bonding in Nanomaterials -Chemical Bonds (types and strength) Intermolecular Forces Molecular and Crystalline Structures, Hierarchical Structures Bulk to Surface transition, surface reconstruction.

### UNIT - II Synthesis and stabilization of nanoparticles

**Nanomaterial Synthesis:-** Chemical routes, Electrochemical methods, Vapor growth, **Thin films methods:** chemical vapor deposition, physical vapor deposition (sputtering, laser ablation), Langmuir-Blodgett growth, **Mechanical methods:** ball milling, mechanical attrition, Sol-gel methods, Special nanomaterials: carbon nanotubes, fullerenes, nanowires, porous silicon, Bio-inspired synthesis Nanocomposite fabrication, Nanolithography, cryochemical synthesis, Stabilization of nanoparticles.



### **UNIT - III Carbon nanotubes and Nanosensors**

**Carbon nanostructures:** Introduction. Fullerenes, C60, C80 and C240 nanostructures. Properties & applications (mechanical, optical and electrical). Functionalization of carbon nanotubes, reactivity of carbon nanotubes. **Nanosensors:** Temperature sensors, smoke sensors, sensors for aerospace and defence. Accelerometer, pressure sensor, night vision system, nano tweezers, nano-cutting tools, integration of sensor with actuators and electronic circuitry biosensors.

### **UNIT - IV Properties and Size dependence of properties**

Chemical, Optical, vibrational, thermal, Electrical, Magnetic Mechanical, Surface and Quantum Confinement effect and Surface reactivity.

### **UNIT – V Applications of nanomaterials and Nanotechnology in nature**

**Applications of nanomaterials:** Applications of nanoparticles in Solar cells-smart materials-molecular electronics- biosensors-various fundamental research, industries, medical field and environmental issues. Biosafety and ethical issue in application of nanoparticles. Toxicity of nano materials.

**Nanotechnology in Nature:** The science behind the nanotechnology in lotus effect-self cleaning property of lotus-gecko footclimbing ability of geckos-water strider-antiwetting property of water striders-spider silk mechanical properties of the spider silk.

### **SUGGESTED READINGS**

1. Br'echignac, C., Houdy., & Lahmani, M. (2007). *Nanomaterials and Nanochemistry*. New York: Springer Berlin Heidelberg.
2. Hosokawa, M., Nogi, K., Naito, M., & Yokoyama, T. (2012). *Nanoparticle Technology Handbook* (II Edition). Elsevier.
3. Theodore, L. (2006). *Nanotechnology: Basic Calculations for Engineers and Scientists*. Hoboken: John Wiley & Sons. Inc., Publication.
4. Introduction to Nanoscience, J. Dutta, H.F. Tibbals and G.L. Hornyak, CRC press, Boca Raton, 2008.
5. Sulabha K. Kulkarni , (2014). *Nanotechnology: Principles and Practices*, Springer Publisher.

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<b>21CHP305A</b>	<b>POLYMER CHEMISTRY</b>	<b>Semester-III</b>
		<b>4H 4C</b>
<b>Instruction Hours/week: L:4 T:0 P:0</b>		<b>Marks: Internal: 40 External: 60 Total:100</b>
<b>External Semester Exam: 3 Hours</b>		

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**Course Objectives**

This course enables the students to

- Understand the basic concepts of polymerization.
- Analyze coordination polymerization and apply the Ziegler-natta catalyst in polymer synthesis.
- Determine the molecular weight of polymers by different methods.
- Analyze the polymer processing and properties of commercial polymers.
- Apply the polymer processing technique to prepare the polymer products.
- Gain knowledge about the commercial polymers and its application.

**Course Outcomes (CO's)**

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

1. Understand the basic concepts of polymerization.
2. Analyse coordination polymerization and apply the Ziegler-natta catalyst in polymer synthesis.
3. Determine the molecular weight of polymers.
4. Analyse polymer processing and properties of commercial polymers.
5. Apply the polymer processing technique to prepare the polymer products.
6. List out the commercial polymers and its application.

**UNIT - I Polymer Basic Concepts**

Monomers, repeat units, degree of polymerization, linear, branched and network polymers. Condensation polymerization: Mechanism of stepwise polymerization. Kinetics and statistics of linear stepwise polymerization. Addition polymerization: Free radical, cationic and anionic polymerization. Polymerization conditions. Polymerization in homogeneous and heterogeneous systems.

**UNIT - II Co-ordination Polymerization**

Kinetics, mono and bimetallic mechanism of co- ordination polymers. Zeigler Natta catalyst, co-polymerization: Block and graft co- polymers, kinetics of copolymerization. Types of co-polymerization. Reactivity ratio.

### **UNIT - III Molecular Weight and Properties**

Polydispersion – average molecular weight concept, number, weight and viscosity average molecular weights. Measurement of molecular weights. Viscosity, light scattering, osmotic and ultracentrifugation methods. Polymer structure and physical properties – crystalline melting point  $T_m$ . The glass transition temperature. Determination of  $T_g$ . Relationship between  $T_m$  and  $T_g$ .

### **UNIT – IV Polymer Processing**

Plastics, elastomers and fibres. Compounding, processing techniques: calendaring, die casting, rotational casting, film casting, injection moulding, blow moulding extrusion, moulding, thermoforming, foaming, reinforcing and fibre spinning.

### **UNIT - V Properties of Commercial Polymers**

Polyethylene, polyvinyl chloride, polyamides, polyesters, phenolic resins, epoxy resins and silicone polymers. Functional polymers, fire retarding polymers and electrically conducting polymers. Biomedical polymers – contact lens, dental polymers, artificial heart, kidney, skin and blood cells.

### **SUGGESTED READINGS:**

1. Billmeyer, F. W. (2003). *Text Book of Polymer Science* (III Edition). New York: John Wiley.
2. Gowariker, V. R., Viswanathan, N. V., & Sreedhar, J. (2015). *Polymer Science* (II Edition). New Delhi: New Age International Private Ltd.
3. Alcock, H. R., Lampe, F. W., & Mark, J. E. (2003). *Contemporary Polymer Chemistry* (III Edition). NJ: Prentice Hall Englewood Cliffs.
4. Flory, P. J. (1953). *Principles of Polymer Chemistry*. New York: Cornell University Press.
5. Odian, G. (2004). *Principles of Polymerization* (IV Edition). New York: John Wiley & Sons.

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**21CHP305B****TEXTILE CHEMISTRY****Semester-III****4H 4C****Instruction Hours/week: L:4 T:0 P:0****Marks: Internal:40 External: 60 Total:100****External Semester Exam: 3 Hours****Course Objectives**

This course enables the students to

- Understand the classification, chemical structure, production, properties and uses of fibers.
- Understand the dyeing process on fibers.
- Analyzes the types of dyes in various applications.
- Evaluate the pollution control in textile industry.
- Apply the various finishing process of fibers.
- Fabricate the material and its dyeing process.

**Course Outcomes (CO's)**

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

1. Understand the classification, chemical structure, production, properties and uses of fibers.
2. Describe the dyeing process on fibers.
3. Classify the types of dyes in various applications.
4. Evaluate the pollution control in textile industry.
5. Illustrate the various finishing process of fibers.
6. Fabricate the material and its dyeing process.

**UNIT- I Fibers**

General classification of fibers-chemical structure, production, properties and uses of the following natural fibers (a) natural cellulose fibers (cotton and jute) (b) natural protein fiber (wool and silk).

Chemical structure, production, properties and uses of the following synthetic fibers.

(i) Manmade cellulosic fibers (Rayon, modified cellulose fibers) (ii) Polyamide fibers (different types of nylons) (iii) Poly ester fibers.

**UNIT- II Dyeing Process**

Impurities in raw cotton and grey cloth, wool and silk- general principles of the removal – scouring – bleaching – desizing – kierboiling- chemicking.

Dyeing - Dyeing of wool and silk –fastness properties of dyed materials – dyeing of nylon, terylene and other synthetic fibres.

### **UNIT- III Finishing**

Finishes given to fabrics- mechanical finishes on cotton, wool and silk, method used in process of mercerizing –anti-crease and anti-shrink finishes –water proofing.

### **UNIT-IV Types of Dyes**

Quinonoid dyes-examples and structure-Anthroquinone and Mordant dyes-synthesis and applications of Alizarin-Phthalocyanin dyes-Copper Phthalocyanin- synthesis and applications.

Diphenylmethane dyes- Auramine-Triphenylmethane dyes-Malachite green, Crystal violet, Pararosaniline-preparation and applications.

Indigo dyes-preparation and application-derivatives of Indigo- synthesis and uses of Indigosol and tetrahaloindigo.

Phthalein dyes-Phenolphthalein- preparation and applications.

Xanthene dyes-Rhodamine B, Fluorescein-Eosin- preparation and applications.

### **UNIT-V Pollution Control in Textile Industry**

Textile effluent-characteristics, effect of untreated effluent, degradability of wastes. Effluent treatment plants-aerated lagoon, photo oxidation process.

### **SUGGESTED READINGS:**

1. Chatwal, R. (2016). *Synthetic Dyes*. Mumbai: Himalayan Publishing House.
2. Robert R Mather and Roger H Wardman (2015). *The Chemistry of Textile fibres*(2<sup>nd</sup> New Edition). New York: RSC Publishing.
3. Rastogi Deepali and Chopra Sheetal (2017). *Textile Science* (I Edition).Hyderabad: Orient Blackswan Private Limited.
4. Krishna Chawla (2016). *Fibrous Materials*. Cambridge University Press.
5. Sharma, B. K. (2016). *Industrial Chemistry*. Krishna Prakashan Media, P,Ltd, Meerut.
6. Jean Hellot (2017) *Art of Dying Wool, Silk and Cotton*, Forgotten Books, Andesite Press.

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		<b>Semester - III</b>	
<b>21CHP305C</b>	<b>INDUSTRIAL CHEMISTRY</b>	<b>4H</b>	<b>4C</b>
<b>Instruction Hours/week: L: 4 T: 0 P: 0 Marks: Internal: 40 External: 60 Total: 100</b>			
<b>External Semester Exam: 3 Hours</b>			

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**Course Objectives**

This course enables the students to

- Understand the role of metals in human body.
- Analyze the physical methods in bioinorganic chemistry, metal biomolecules interactions, complexes, and drug discovery.
- Analyse the binding of metal ions and complexes to biomolecules.
- Analyze the complexes and chelating agents.
- Evaluate the drug discovery and design tools and its importance in clinical trials.
- Apply these parameters to discover new pharmacokinetic molecules.

**Course Outcomes (CO's)**

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

1. List out the role of metals in human body.
2. Analyse the physical methods in bioinorganic chemistry, metal biomolecules interactions, complexes, and drug discovery.
3. Analyse the binding of metal ions and complexes to biomolecules.
4. Compare the complexes and chelating agents.
5. Apply the fundamental knowledge in drug discovery and design.
6. Apply these parameters to discover new pharmacokinetic molecules.

**UNIT – I Metals in the Human Body**

General principles - the elements in the human body - biological significance, storage and transport of Fe, Zn, Cu, Mo, Co, Cr, V and Ni - metal functions in metalloproteins - metallo enzyme functions – Photosystems - Phorphyrins -supplying elements to the body - metals and human health.

**UNIT – II Physical Methods in Bioinorganic Chemistry**

X-ray methods - magnetic resonance methods - mossbauer spectroscopy - magnetic measurements -other instrumental methods  
-atomic force microscopy - fast and time-resolved methods - stopped-flow kinetic methods  
- flash photolysis - time-resolved crystallography.

### **UNIT – III Binding of Metal Ions and Complexes to Biomolecules**

Nucleic acid structures - fundamental interactions with nucleic acids - binding interactions of tris(phenanthroline) metal complexes with DNA - techniques to monitor binding - applications of metal complexes that bind to nucleic acids -biopolymer promoted metal ligand interactions.

### **UNIT - IV Complexes and Chelating Agents**

Labile and inert complexes - metal-ligand selectivity-HSAB approach-chelate effect and Irving-William series -survey of metals used for diagnosis and chemotherapy-radiodiagnostic agents-Magnetic Resonance Imaging (MRI) - gold and other metal phosphines-main-group and transition metal compounds - miscellaneous metals in medicine-chelating agents and therapy - EDTA- evolution, chemical properties, *in vivo* chelation of radionuclides, dosage and toxicity .

### **UNIT - V Drug Discovery and Design**

Outline- therapeutic index, chemotherapeutic index, structure- activity relationship (SAR) and quantitative structure-activity relationship (QSAR)-Factors governing drug design-computer aided drug design-cancer chemotherapy-bioinorganic chemistry (DNA binding) of platinum anticancer drugs (cisplatin and carboplatin)-mechanism of action studies-clinical trials and their significance- production and quality control- patent protection.

### **SUGGESTED READINGS:**

1. Taylor, D. M., & Williams, D. R. (1995). *Trace Element Medicine and Chelation Therapy* (I Edition). United Kingdom: The Royal Society of Chemistry.
2. Ashutosh Kar, (2000). *Medicinal Chemistry*. New Delhi: New Age International Publishers.
3. Gareth Thomas, (2000). *Medicinal Chemistry*. United Kingdom: John-Wiley & Sons Ltd.
4. Bertini, I., Gray, H. B., Lippard, S. J., & Valentine, J. S. (1994). *Bioinorganic Chemistry*. California: University Science books.
5. Roat-Malone, R. M. (2002). *Bioinorganic Chemistry*. NJ: John Wiley & Sons. Inc.
6. Das, A.K. (2015). *Bio-inorganic Chemistry*, Books & Allied Pvt. Ltd., Kolkatta.

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**Semester-III**

**21CHP311                      PHYSICAL CHEMISTRY PRACTICAL-I                      4H    2C**  
**(MOLECULAR WEIGHT DETERMINATION AND CONDUCTOMETRIC TITRATIONS)**

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**Instruction Hours/week: L: 0 T: 0 P: 4    Marks: Internal: 40 External: 60 Total: 100**  
**External Semester Exam: 6 Hours**

**Course Objectives**

This course enables the students to

- Determine the heat of solution, determination of molecular weight and distribution coefficient.
- Apply the basic concepts of conductometric titrations to determine the ionic strength.
- Understand the various laws in electrochemistry.
- Apply the conductometric method for the solutions and measure its conductivity.
- Handle the conductivity meter, spectrophotometer.
- Evaluate distribution co-efficients influence the solubility of various systems.

**Course Outcomes (CO's)**

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

1. Determine the heat of solution, determination of molecular weight and distribution coefficient.
2. Apply the basic concepts of conductometric titrations to determine the ionic strength.
3. Understand the various laws in electrochemistry.
4. Classify the conductometric method for the solutions and measure its conductivity.
5. Handle the conductivity meter, spectrophotometer.
6. Analyse the distribution co-efficient influence the solubility of various systems.

**Contents**

1. Determination of the heat of solution of a substance by solubility method.
2. Determination of the solubility of  $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$  in water by gravimetric method at several temperatures.
3. Determination of neutralization enthalpy of HCl and  $\text{CH}_3\text{COOH}$  by NaOH.
4. Determination of hydrolysis constant of aniline hydrochloride.
5. Determination of dissociation constant of a weak acid by pH metric titration.
6. pH metric titration of mixture of weak acid and strong acid against strong base.
7. Setting up of various cells and measurement of their values, Examples: Zn /0.1M  $\text{ZnSO}_4$ /



KCl / Hg<sub>2</sub>Cl<sub>2</sub> / Hg / Ag / AgCl / 0.1 M KCl / Hg<sub>2</sub>Cl<sub>2</sub> / Hg / Hg<sub>2</sub>Cl<sub>2</sub> / KCl / 0.1 M CuSO<sub>4</sub> / Cu.

8. Determination of standard electrode potentials, activity coefficient and acid dissociation constant from Hamed Cell e.m.f's, (Hamed Cell is Pt / H<sub>2</sub> / HCl/AgCl, AgBr).

9. Determination of equivalent conductance, degree of dissociation and dissociation constant of a weak acid.

10. Determination of Equivalent conductance, degree of dissociation and dissociation constant of a strong electrolyte.

11. Verification of Debye-Huckel Onsager equation.

12. Verification of Ostwald dilution law.

13. Verification of Kohlraush law for weak electrolytes.

14. Conductometric titration of a mixture of a weak acid and strong acid against a strong base.

15. Determination of the solubility of a sparingly soluble salt.

16. Conductometric titration: Acid-base and precipitation titrations including mixture of halides.

### **SUGGESTED READINGS:**

1. Lepse, P. A., & Lyle B. P., (1986). *Lab Manual for Lingren's Essentials of Chemistry*. New Delhi: Prentice Hall.
2. Pandey, O. P, Bajpai, D. N., & Giri, S. (2001). *Practical Chemistry* (VIII Edition). New Delhi: S. Chand Publications.
3. Santi Rajan Palit and Sadhan Kumar, (1971). *Practical Physical Chemistry* (I Edition). Calcutta: Joy Publishers.
4. Siddhiqui, Z. N. (2002). *Practical Industrial Chemistry* (I Edition). New Delhi: Anmol Publications Pvt. Ltd.
5. Thomas, A.O, (2003). *Practical Chemistry*. Cannanore: Scientific Book Center.
6. Venkateswaran, V., Veeraswamy, R., & Kulandaivelu, A. R. (2004). *Basic Principles of Practical Chemistry* (II Edition). New Delhi: S. Chand Publications.
7. Srivastava.T.N., & Kamboj. P.C., University Practical Chemistry (2013). New Delhi. Milestone Publishers and Distributors.

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21CHP312	PHYSICAL CHEMISTRY PRACTICAL- II (CHEMICAL KINETICS AND POTENTIOMETRIC TITRATIONS)	Semester-III 4H 2C
Instruction Hours/week: L:0 T:0 P:4		Marks: Internal:40 External: 60 Total:100
External Semester Exam: 3 Hours		

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### Course Objectives

This course enables the students to

- Understand the principles of electrochemistry and determination EMF.
- Know the applications of chemical kinetics and potentiometric titrations.
- Analyze the principles of adsorption process.
- Apply the concepts to handle the potentiometer, electrodes and spectrophotometer.
- Analyze the chemical kinetics in various preparation organic/inorganic compounds.
- Evaluate the metal concentration in water samples using adsorption technique.

### Course Outcomes (CO's)

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

1. Understand about the principles of electrochemistry and determination EMF.
2. Know the basic needs of chemical kinetics and potentiometric titrations.
3. Appreciate the principles about adsorption process.
4. Demonstrate the setup of the potentiometer and spectrophotometers.
5. Determine the chemical kinetics parameters in various preparation organic/inorganic compounds.
6. Test the metal concentration in water samples using adsorption technique.

### Contents

Electromotive force determination of standard potentials of Cu, Zn and Ag.

Determination of pH and pKa values using hydrogen and quinhydrone electrodes and glass electrode pH meter- potentiometric acid-base titrations.

Determination of formal redox potential of a redox system and redox titrations.

Determination of solubility product of a sparingly soluble salt concentration cell and chemical cell.

Determination of activity co-efficients from emf data. Precipitation titration of a mixture of halides.

Chemical kinetics:

- i. Evaluation of Arrhenius parameters using acid hydrolysis of an ester.

- ii. Base catalyzed hydrolysis of an ester conductometrically.
- iii. Rate of reaction between persulphate and iodide ions study of salt over the persulphate- iodide reaction.

Evaluation of catalytic constants for weak acids and verification of Bronsted catalysis law.

Adsorption Experiments:

Adsorption of oxalic acid and acetic acid on activated charcoal-Fruendlich isotherm.

### **SUGGESTED READINGS:**

1. Lapse, P. A., & Lyle B. P., (1986). *Lab Manual for Lingren's Essentials of Chemistry*. New Delhi: Prentice Hall.
2. Pandey, O. P, Bajpai, D. N., & Giri, S. (2001). *Practical Chemistry* (VIII Edition). New Delhi: S. Chand Publications.
3. Santi Rajan Palit and Sadhan Kumar, (1971). *Practical Physical Chemistry* (I Edition). Calcutta: Joy Publishers.
4. Siddhiqui, Z. N. (2002). *Practical Industrial Chemistry* (I Edition). New Delhi: Anmol Publications Pvt. Ltd.
5. Thomas, A.O, (2003). *Practical Chemistry*. Cannanore: Scientific Book Center.
6. Venkateswaran, V., Veeraswamy, R., & Kulandaivelu, A. R. (2004). *Basic Principles of Practical Chemistry* (II Edition). New Delhi: S. Chand Publications

**M.Sc. Chemistry**

**2021-2022**

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<b>21CHP491</b>	<b>PROJECT AND VIVA-VOCE</b>	<b>Semester-IV</b>
		<b>30H 15C</b>
<b>Instruction Hours/week:L: 0 T: 0 P: 30 Marks: Internal: 80 External: 120 Total:100</b>		

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