



**SACRED HEART COLLEGE (AUTONOMOUS)  
THEVARA, KOCHI – 682013  
KERALA**

**CURRICULUM AND SYLLABUS  
of  
M.Sc. CHEMISTRY  
(PG CREDIT SEMESTER SYSTEM)**

INTRODUCED FROM 2020-21 ADMISSION ONWARDS

**Board of Studies in Chemistry  
Sacred Heart College (Autonomous)  
Thevara**

## PREFACE

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

Chemistry is beyond the science of mere observation and understanding of nature. In the words of James Watson, a 1962 Nobel Laureate in Physiology or Medicine, put it well: “Life is simply a matter of chemistry”. It is with this vision we revised the syllabi for the PG courses, and also we followed the PG Guidelines which was prepared by the dean faculty. The revised syllabi will be implemented with effect from the academic year 2020-21 admission onwards.

The PG Board of Studies in Chemistry was entrusted with the duty of preparing the revised curricula and syllabi for the two M.Sc. Programmes in Chemistry currently approved by the Mahatma Gandhi University. The BoS has taken keen interest in collecting expert opinion from the renowned experts in the field as well as from the faculties of the affiliated colleges handling the subjects. We have also referred to the syllabi of various other Universities such as that of Cochin University of Science and Technology, Calicut University, Pune University, Delhi University besides, that of University Grants Commission and offered in the affiliated colleges.

The BoS prepared draft proposals of revised curricula and syllabi for the two M.Sc. Programmes in Chemistry keeping the Credit and Semester System. The syllabus has been set with an objective of training the students in all the fundamentals of the subject along with good practical exposure. Most of the advanced topics have been incorporated in the fourth semester. In view of creating research aptitude in students, BoS has decided to give sufficient time for project work, at least three months, and as far as possible send the students in reputed research centres/Universities in and outside the state for doing their project. Since specific time is not allotted for project work in the academic calendar, students can go for project after their final semester examinations.

The BoS feels that appreciable updating could be done in keeping with the current developments and trends in chemistry education. The task of preparing the Curricula and Syllabi and bringing it out in the present form was not a simple task but it was possible with dedicated efforts and wholehearted support and involvement of all the members of the faculty and BoS. I would like to express my sincere thanks to all my fellow members of the BOS and faculty for all their whole hearted time-bound help, cooperation and encouragement. I also express my sincere gratitude to Prof. S. Suganan (CUSAT), Prof.(Rtd.) K. K Vijayan (Calicut University), Prof. Abraham Joseph (Calicut University), Dr. M. K Muraleedharan Nair (Maharajas College), Dr. Mahesh Hariharan (IISER – TVM) and Dr. Pramod Padmanabhan (IISER – Pune) for their meaningful contributions.

**Dr. V. S. Sebastian**

**Chairman**

**PG & UG Board of Studies**

**Sacred Heart College (Autonomous). Thevara.**

**BOARD OF STUDIES IN CHEMISTRY****Sacred Heart College (Autonomous)****Thevara, Kochi, Kerala**

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4		<i>Expert to be nominated by the Vice Chancellor from a panel of six recommended by the College Principal</i>
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6	<b>Dr. Kochubaby Manjooran,</b> Manager, Energy and Environment Division, Kochi Refineries Ltd., Ambalamukal, Ernakulam Dist.	<i>Representative from industry, corporate – sector or allied area.</i>
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### **Programme Outcomes (POs) for the Postgraduate Students of Sacred Heart College, Kochi**

At the end of the programme, the student should be able to:

<b>PO 1</b>	Exercise their critical thinking in creating new knowledge leading to innovation, entrepreneurship and employability.
<b>PO 2</b>	Effectively communicate the knowledge of their study and research in their respective disciplines to their stakeholders and to the society at large.
<b>PO 3</b>	Make choices based on the values upheld by the institution, and have the readiness and know-how to preserve the environment and work towards sustainable growth and development.
<b>PO 4</b>	Develop an ethical view of life and have a broader (global) perspective transcending the provincial outlook.
<b>PO 5</b>	Explore new knowledge independently for the development of the nation and the world and are able to engage in a lifelong learning process.

### **Programme Specific Outcomes (PSOs) of MSc Chemistry**

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

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

## General Information

### 1. SCOPE

**1.1** These regulations provided herein shall apply to all post-graduate programmes, conducted by Sacred Heart College (S.H. College), Thevara with effect from the academic year 2020-2021 admission onwards.

### 2. DEFINITIONS

**2.1** ‘**Academic Committee**’ means the Committee constituted by the principal under this regulation to monitor the running of the Post-Graduate programmes under the Choice Based Credit System (CBCS-PG).

**2.2** ‘**Programme**’ means the entire course of study and examinations.

**2.3** ‘**Duration of Programme**’ means the period of time required for the conduct of the programme. The duration of post-graduate programme shall be of 4 semesters.

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

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

**2.6** ‘**Credit**’ (Cr) of a course is the numerical value assigned to a paper according to the relative importance of the content of the syllabus of the programme.

**2.7** ‘**Programme Credit**’ means the total credit of the PG Programmes, ie; **80 credits**.

**2.8** ‘**Programme Core course**’ Programme Core course means a course that the student admitted to a particular programme must successfully complete to receive the Degree and which cannot be substituted by any other course.

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

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

**2.11** ‘**Plagiarism**’ Plagiarism is the unreferenced use of other authors’ material in dissertations and is a serious academic offence.

- 2.12 ‘Tutorial’** Tutorial means a class to provide an opportunity to interact with students at their individual level to identify the strength and weakness of individual students.
- 2.13 ‘Seminar’** seminar means a lecture expected to train the student in self-study, collection of relevant matter from the books and Internet resources, editing, document writing, typing and presentation.
- 2.14 ‘Evaluation’** means every course shall be evaluated by 25% internal assessment and 75% external assessment.
- 2.15 ‘Repeat course’** is a course that is repeated by a student for having failed in that course in an earlier registration.
- 2.16 ‘Audit Course’** is a course for which no credits are awarded.
- 2.17 ‘Department’** means any teaching Department offering a course of study approved by the college / Institute as per the Act or Statute of the University.
- 2.18 ‘Parent Department’** means the Department which offers a particular Post graduate programme.
- 2.19 ‘Department Council’** means the body of all teachers of a Department in a College.
- 2.20 ‘Faculty Advisor’** is a teacher nominated by a Department Council to coordinate the continuous evaluation and other academic activities undertaken in the Department.
- 2.21 ‘College Co-ordinator’** means a teacher from the college nominated by the College Council to look into the matters relating to CBCS-PG System
- 2.22 ‘Letter Grade’** or simply ‘**Grade**’ in a course is a letter symbol (S, A, B, C, D, etc.) which indicates the broad level of performance of a student in a course.
- 2.23** Each letter grade is assigned a ‘**Grade point**’ (GP) which is an integer indicating the numerical equivalent of the broad level of performance of a student in a course.
- 2.24 ‘Credit point’** (CP) of a course is the value obtained by multiplying the grade point (GP) by the Credit (Cr) of the course  $CP=GP \times Cr$ .
- 2.25 ‘Extra credits’** are additional credits awarded to a student over and above the minimum credits required for a programme for achievements in co-curricular activities carried out outside the regular class hours as directed by the College/ department.
- 2.26 ‘Semester Grade point average’** (SGPA) is the value obtained by dividing the sum of credit points (CP) obtained by a student in the various courses taken in a semester by the total number of credits taken by him/her in that semester. The grade points shall be rounded off to two decimal places. SGPA determines the overall performance of a student at the end of a semester.
- 2.27 ‘Cumulative Grade Point Average’** (CGPA) is the value obtained by dividing the sum of credit



points in all the courses taken by the student for the entire programme by the total number of credits and shall be rounded off to two decimal places.

**2.28 ‘Grace Marks’** means marks awarded to course/s, as per the orders issued by the college from time to time, in recognition of meritorious achievements in NCC/NSS/Sports/Arts and cultural activities.

**2.29 ‘Words and expressions’** used and not defined in this regulation but defined in the Mahatma Gandhi University Act and Statutes shall have the meaning assigned to them in the Act and Statute.

### **3. ACADEMIC COMMITTEE**

3.1 There shall be an Academic Committee constituted by the principal to manage and monitor the working of (CBCS-PG) 2020.

3.2 The Committee consists of

- (a) The principal
- (b) The vice principal
- (c) Deans of the faculties of science, arts and commerce
- (d) The Controller of Examinations
- (e) IQAC –Co-ordinator
- (f) The superintendent of the college

### **4. PROGRAMME STRUCTURE**

4.1 Students shall be admitted into post graduate programmes under the various faculties.

4.2 The programme shall include two types of courses, Program Core (C) courses and Program Elective (E) Courses. There shall be a Program Project (D) with dissertation to be undertaken by all students. The Programme will also include assignments, seminars, practical (P), viva (V), study tour etc., if they are specified in the Curriculum

4.3 There shall be various groups of four Programme Elective courses for a programme such as Group A, Group B etc. for the choice of students subject to the availability of faculty and infrastructure in the institution and the selected group shall be the subject of specialization of the programme.

4.4 Project work

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

4.4.2 Project work shall be carried out under the supervision of a teacher in the concerned department.

- 4.4.3. A candidate may, however, in certain cases be permitted to work on the project in an industrial / Research Organization/ Institute on the recommendation of the Supervisor.
- 4.4.4 There should be an internal assessment and external assessment for the project work in the ratio 1:3
- 4.4.5 The external evaluation of the Project work is followed by presentation of work including dissertation and Viva-Voce.
- 4.4.6 The mark and credit with grade awarded for the program project should be entered in the grade card issued by the college.
- 4.5. Assignments: Every student shall submit one assignment as an internal component for every course.
- 4.6 Seminar Lecture: Every PG student may deliver one seminar lecture as an internal component for every course. The seminar lecture is expected to train the student in self-study, collection of relevant matter from the books and Internet resources, editing, document writing, typing and presentation.
- 4.7 Every student shall undergo two class tests as an internal component for every course.
- 4.8 The attendance of students for each course shall be another component of internal assessment.
- 4.9 Comprehensive Viva-voce shall be conducted at the end of the programme which covers questions from all courses in the programme as per the syllabus.

## 5. ATTENDANCE

- 5.1 The minimum requirement of aggregate attendance during a semester for appearing the end semester examination shall be 75%. Condonation of shortage of attendance to a maximum of 10 days in a semester subject to a maximum of two times during the whole period of Post Graduate programme may be granted by the College as forwarded on the recommendation by the class teacher/HOD.
- 5.2 If a student represents the college in University, State or Nation in Sports, NCC, NSS or Cultural or any other officially sponsored activities such as College union / University union activities, he/she shall be eligible to claim the attendance for the actual number of days participated subject to a maximum of 10 days in a Semester based on the specific recommendations of the Head of the concerned Department and Principal of the College.
- 5.3 A student who does not satisfy the requirements of attendance shall not be permitted to take the end Semester examinations.
- 5.4 Those students who are not eligible even with condonation of shortage of attendance shall

repeat the course along with the next batch

## 6. BOARD OF STUDIES AND COURSES

- 6.1 The Board of Studies concerned shall design all the courses offered in the PG programme. The Boards shall design and introduce new courses, modify or re-design existing courses and replace any existing courses with new/modified courses to facilitate better exposures and training for the students.
- 6.2 The syllabus of a course shall include the title of the course, contact hours, the number of credits and reference materials.
- 6.3 Each course shall have an alpha numeric code number which includes abbreviation of the subject in two letters, the semester number, the code of the course and the serial number of the course ('C' for Program Core course, 'E' for Program Elective course, 'O' for Open Elective course, 'P' for Practical and 'D' for Project/ Dissertation and 'V' for Comprehensive Viva voce).
- 6.4 Every Programme conducted under Choice Based Credit System shall be monitored by Academic committee and the College Council.

## 7. REGISTRATION

- 7.1 A student shall be permitted to register for the programme at the time of admission. The duration of the PG Programme shall be 4 semesters.
- 7.2 A student who registered for the course shall complete the course within a period of 8 continuous semesters from the date of commencement of the programme.

## 8. ADMISSION

- 8.1 The admission to all PG programmes shall be as per the rules and regulations of the college.
- 8.2 The eligibility criteria for admission shall be as announced by the college from time to time.
- 8.3 There shall be provision for inter collegiate and inter University transfer within a period of two weeks from the date of commencement of the semester.
- 8.4 There shall be provision for credit transfer subject to the conditions specified by the Board of Studies concerned.

## 9. ADMISSION REQUIREMENTS

- 9.1 Candidates for admission to the first semester of the PG programme through CBCS shall be required to have passed an appropriate Degree Examination of Mahatma Gandhi University as

specified or any other examination of any recognized University or authority accepted by the Academic council of the college as equivalent thereto.

9.2 The candidate must forward the enrolment form to the Controller of Examinations of the college through the Head of the Department.

9.3 The candidate has to register all the courses prescribed for the particular semester. Cancellation of registration is applicable only when the request is made within two weeks from the time of admission.

9.4 Students admitted under this programme are governed by the Regulations in force.

**10. PROMOTION:** A student who registers for the end semester examination shall be promoted to the next semester

## **11. EXAMINATIONS**

11.1 There shall be an external examination at the end of each semester.

11.2 The answers must be written in **English** except for those coming under Faculty of languages.

11.3 Practical examinations shall be conducted by the college at the end of the semesters as per the syllabus.

11.4 Project evaluation and Comprehensive Viva -Voce shall be conducted as per the syllabus. Practical examination, Project evaluation and Comprehensive Viva-Voce shall be conducted by two external examiners.( For professional courses, one examiner can be opted from the same college itself)

11.5 There shall be one end-semester examination of 3 hours duration in each lecture based course (Theory).

11.6 A question paper may contain multiple choice /objective type, short answer type/annotation, short essay type questions/problems and long essay type questions. Different types of questions shall have different marks, but a general pattern may be followed by the Board of Studies.

## **12. EVALUATION AND GRADING**

**12.1 Evaluation:** The evaluation scheme for each course shall contain two parts; (a) internal evaluation (ISA) and (b) end semester evaluation (ESA). 25 marks shall be given to internal evaluation and 75 marks to external evaluation so that the ratio between internal and external mark is 1:3. Both internal and external evaluation shall be carried out in mark system. Both internal and external marks are to be mathematically rounded to the nearest integer.

**12.2 Internal evaluation:** The internal evaluation shall be based on predetermined transparent system involving periodic written tests, assignments, seminars/viva/field survey and attendance in respect of theory courses and based on written tests, lab skill/records/viva and attendance in respect of practical courses. The marks assigned to various components for internal evaluation is as follows.

### 12.3 Components of Internal Evaluation

All the components of the internal evaluation are mandatory

**a) For Theory**

Components	Marks
Assignment	5
Seminar/Quiz/Field survey /Viva etc.	5
Attendance	5
Two Test papers (2 x 5)	10
<b>Total</b>	<b>25</b>

**b) For Practical**

Components	Marks
Attendance	5
Written/Lab test	5
Laboratory Involvement/ Record*	10
Viva	5
<b>Total</b>	<b>25</b>

\*Marks awarded for Record should be related to number of experiments recorded

**c) For Project**

Components	Marks
Topic/Area selected	2
Experimentation/Data collection	5
Punctuality	3
Compilation	5
Content	5
Presentation	5
<b>Total</b>	<b>25</b>

## 12.4 Evaluation of Attendance

% of attendance	Mark
Above 90%	5
Between 85 and < 90	4
Between 80 and below 85	3
Between 76 and below 80	2
75	1

## Assignment

Components	Marks
Punctuality	1
Content	2
Conclusion	1
Reference/Review	1
<b>Total</b>	<b>5</b>

## Seminar

Components	Marks
Content	2
Presentation	2
Reference/Review	1
<b>Total</b>	<b>5</b>

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

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

**12.7 External Evaluation:** The external examination in theory courses shall be conducted by the college with question papers set by external experts/ question bank. The evaluation of the answer

scripts shall be done by the examiners based on a well-defined scheme of evaluation given by the question paper setters. The external evaluation shall be done immediately after the examination preferably through the centralised valuation.

**12.8** The question paper should be strictly on the basis of model question paper set by BoS with due weightage for each module of the course and there shall be a combined meeting of the question paper setters and experts for scrutiny for finalisation of question paper. Each set of question should be accompanied by its scheme of valuation.

**12.9** For all courses (theory & practical), Letter grades and grade point are given on a 10-point scale based on the total percentage of marks, (ISA+ESA) as given below:-

Percentage of Marks	Grade	Grade Point (GP)
95 and above	O Outstanding	10
85 to below 95	A <sup>+</sup> Excellent	9
75 to below 85	A Very Good	8
65 to below 75	B <sup>+</sup> Good	7
55 to below 65	B Above Average	6
45 to below 55	C Average	5
40 to below 45	D Pass	4
Below 40	F Fail	0
	Ab Absent	0

*Grades for the different semesters and overall programme are given based on the corresponding GPA as shown below:*

GPA	Grade
Equal to 9.5 and above	<i>O Outstanding</i>
Equal to 8.5 and below 9.5	<i>A+ Excellent</i>
Equal to 7.5 and below 8.5	<i>A Very Good</i>
Equal to 6.5 and below 7.5	<i>B+ Good</i>
Equal to 5.5 and below 6.5	<i>B Above Average</i>
Equal to 4.5 and below 5.5	<i>C Average</i>
Equal to 4.0 and below 4.5	<i>D Pass</i>
Below 4.0	<i>F Failure</i>

**12.10** A separate minimum of 40% marks (D grade) required for a pass for both internal evaluation and external evaluation for every course.

**12.11** A candidate who has not secured minimum marks/credits in internal examinations can re-do the same registering along with the end semester examination for the same semester, subsequently.

**12.12** A student who fails to secure a minimum marks/grade for a pass in a course will be permitted to write the examination along with the next batch.

**There will be no improvement examinations**

**12.13** After the successful completion of a semester, Semester Grade Point Average (SGPA) of a student in that semester is calculated using the formula given below. For the successful completion of semester, a student should pass all courses and score a minimum SGPA of 4.0. However, a student is permitted to move to the next semester irrespective of her/his SGPA.

**Credit Point (CP)** of a course is calculated using the formula

$CP = Cr \times GP$ , where Cr = Credit; GP = Grade point

**Semester Grade Point Average (SGPA)** of a Semester is calculated using the formula

$SGPA = TCP/TCr$ , where

$TCP = \text{Total Credit Point of that semester} = \sum_1^n CP_i$ ;

$TCr = \text{Total Credit of that semester} = \sum_1^n Cr_i$

Where  $n$  is the number of courses in that semester

**Cumulative Grade Point Average (CGPA)** of a Programme is calculated using the formula

$CGPA = \frac{\sum(TCP \times TCr)}{\sum TCr}$  GPA shall be round off to two decimal places

**12.14 PATTERN OF QUESTIONS**

Questions shall be set to assess knowledge acquired, standard, application of knowledge, application of knowledge in new situations, critical evaluation of knowledge and the ability to synthesize knowledge. The question setter shall ensure that questions covering all skills are set. He/She shall also submit a detailed scheme of evaluation along with the question paper.

A question paper shall be a judicious mix of, multiple /objective ,short answer type, short essay type / problem solving type and long essay type questions.



**Pattern of questions for external examination for theory paper**

Type of Questions	Total no. of questions	Number of questions to be answered	Marks of each question	Total marks
Section A – Short Answer	12	8	2	16
Section B- Short essay/ Problems	10	7	5	35
Section C- Long essay	4	2	12	24
	<b>26</b>	<b>17</b>		<b>75</b>

Pattern of questions for external examination of practical papers will be decided by Practical exam board chairman as per the guidelines of Board of Studies.

**13. GRADE CARD**

The colleges under its seal shall issue to the students, a grade card on completion of each semester, which shall contain the following information.

- a) Name of the College
- b) Title of the Postgraduate Programme
- c) Name of the Semester
- d) Name and Register Number of the student
- e) Code, Title, Credits and Max. Marks (Internal, External & Total) of each course (theory & Practical) in the semester.
- f) Internal, External and Total Marks awarded, Grade, Grade point and Credit point in each course in the semester
- g) The total credits, total marks (Max. & Awarded) and total credit points in the semester
- h) Semester Grade Point Average (SGPA) and corresponding Grade.
- i) Cumulative Grade Point Average (CGPA)
- j) The final Mark cum Grade Card issued at the end of the final semester shall contain the details of all courses (theory & practical) taken during the final semester examination and shall include the final grade/marks scored by the candidate from 1st to 3rd semester, and the overall

grade/marks for the total programme.

#### **14. AWARD OF DEGREE**

The successful completion of all the courses with 'D' grade (40%) shall be the minimum requirement for the award of the degree

#### **15. MONITORING COMMITTEE**

There shall be a Monitoring Committee constituted by the principal consisting of faculty advisors, HOD, a member from teacher learning evaluation committee (TLE) and college coordinator to monitor the internal evaluations conducted by college. The Course teacher, Faculty Advisor, and the College Coordinator should keep all the records of the internal evaluation, for at least a period of two years, for verification.

#### **16. GRIEVENCE REDRESSAL MECHANISM**

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

**Level 1:** At the level of the concerned course teacher

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

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

#### **17. TRANSITORY PROVISION**

Notwithstanding anything contained in these regulations, the Principal shall, for a period of three year from the date of coming into force of these regulations, have the power to provide by order that these regulations shall be applied to any programme with such modifications as may be necessary

#### **18. REPEAL**

The Regulations now in force in so far as they are applicable to programmes offered by the college and to the extent they are inconsistent with these regulations are hereby repealed. In the case of any inconsistency between the existing regulations and these regulations relating to the Choice Based Credit System in their application to any course offered in the College, the latter shall prevail.

## PROGRAMME STRUCTURE

Course Code	Course Title	Credits	Hours / Week	Hour / Sem.	Examination		
					ESE Duration	ESE Max. Marks	CIA Max. Marks
<b>SEMESTER I</b>							
20P1CHET01	Inorganic Chemistry - I	4	4	72	3 Hrs.	75	25
20P1CHET02	Basic Organic Chemistry	4	4	72	3 Hrs.	75	25
20P1CHET03	Physical Chemistry - I	3	3	54	3 Hrs.	75	25
20P1CHET04	Quantum Chemistry & Group Theory	4	4	72	3 Hrs.	75	25
20P2CHEP01	Inorganic Chemistry Practical - I	-	3	54	Examination at the end of Sem II		
20P2CHEP02	Organic Chemistry Practical - I	-	3	54	Examination at the end of Sem II		
20P2CHEP03	Physical Chemistry Practical - I	-	4	72	Examination at the end of Sem II		
	<b>Total</b>	<b>15</b>	<b>25</b>	<b>450</b>			
<b>SEMESTER II</b>							
20P2CHET05	Inorganic Chemistry - II	4	4	72	3 Hrs.	75	25
20P2CHET06	Organic Reaction Mechanism	4	4	72	3 Hrs.	75	25
20P2CHET07	Physical Chemistry - II	3	3	54	3 Hrs.	75	25
20P2CHET08	Theoretical & Computational Chemistry	4	4	72	3 Hrs.	75	25
20P2CHEP01	Inorganic Chemistry Practical - I	3	3	54	6 Hrs.	75	25
20P2CHEP02	Organic Chemistry Practical - I	3	3	54	6 Hrs.	75	25
20P2CHEP03	Physical Chemistry Practical - I	3	4	72	6 Hrs.	75	25
	<b>Total</b>	<b>24</b>	<b>25</b>	<b>450</b>			
<b>SEMESTER III</b>							
20P3CHET09	Inorganic Chemistry - III	4	4	72	3 Hrs.	75	25
20P3CHET10	Organic Syntheses	4	4	72	3 Hrs.	75	25
20P3CHET11	Physical Chemistry - III	4	4	72	3 Hrs.	75	25
20P3CHET12	Spectroscopic Methods in Chemistry	3	3	54	3 Hrs.	75	25
20P4CHEP04	Inorganic Chemistry Practical – II	-	3	54	Examination at the end of Sem IV		
20P4CHEP05	Organic Chemistry Practical – II	-	3	54	Examination at the end of Sem IV		
20P4CHEP06	Physical Chemistry Practical - II	-	4	72	Examination at the end of Sem IV		
	<b>Total</b>	<b>15</b>	<b>25</b>	<b>450</b>			
<b>SEMESTER IV</b>							
20P4CHET13EL	Advanced Inorganic Chemistry	4	5	90	3 Hrs.	75	25
20P4CHET14EL	Advanced Organic Chemistry	4	5	90	3 Hrs.	75	25
20P4CHET15EL	Advanced Physical Chemistry	4	5	90	3 Hrs.	75	25
20P4CHEP04	Inorganic Chemistry Practical – II	3	3	54	6 Hrs.	75	25
20P4CHEP05	Organic Chemistry Practical – II	3	3	54	6 Hrs.	75	25
20P4CHEP06	Physical Chemistry Practical – II	3	4	72	6 Hrs.	75	25
20P4CHECV	Comprehensive Subject Viva Voce	2	-	-	30 min	100	-
20P4CHEPJ	Project Viva	3	-	-	30 min	75	25
	<b>Total</b>	<b>26</b>	<b>25</b>	<b>450</b>			

## SEMESTER I

## 20P1CHET01: INORGANIC CHEMISTRY-I

Credits: 4

Contact Lecture Hours: 72

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

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

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

- 1.1 Hapto nomenclature of organometallic compounds, organometallic compounds with linear *pi*-donor ligands-olefins, acetylenes, dienes and allyl complexes-synthesis, structure and bonding.
- 1.2 Synthesis and structure of complexes with cyclic *pi*-donors, metallocenes and cyclic arene complexes, bonding in ferrocene and dibenzenechromium, carbene and carbyne complexes.
- 1.3 **Metal carbonyls: CO as a  $\pi$ -bonding ligand, synergism, preparation, properties, structure and bonding of simple mono and binuclear metal carbonyls, metal nitrosyls, metal cyanides and dinitrogen complexes. Polynuclear metal carbonyls with and without bridging. Carbonyl clusters - LNCCS and HNCCS, Isoelectronic and isolobal analogy, Wade-Mingos rules, cluster valence electrons. IR spectral studies of bridging and non-bridging CO ligands.**

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

- 2.1 **Substitution reactions - nucleophilic ligand substitution, nucleophilic and electrophilic attack on coordinated ligands.**
- 2.2 **Addition and elimination reactions - 1,2 additions to double bonds, carbonylation and decarbonylation, Oxidative addition - concerted addition, S<sub>N</sub>2, radical and ionic mechanisms. Reductive elimination- binuclear reductive elimination and  $\sigma$ -bond metathesis. Oxidative**

coupling and reductive decoupling. Insertion (migration) and elimination reactions – insertions of CO and alkenes, insertion into M–H versus M–R,  $\alpha$ ,  $\beta$ ,  $\gamma$  and  $\delta$  eliminations.

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

### Unit 3: Catalysis by Organometallic Compounds (18 Hrs)

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

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

3.3 Hydroformylation of olefins using cobalt or rhodium catalyst.

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

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

3.6 Olefin methathesis - synthesis gas based reactions, photodehydrogenation catalyst (“Platinum Pop”). Olefin methathesis, photodehydrogenation catalyst (“Platinum Pop”). Palladium catalysed oxidation of ethylene-the Wacker process.

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

3.8 Asymmetric catalysis - Asymmetric hydrogenation, isomerisation and epoxidation.

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

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

### Unit 4: Bioinorganic Compounds (18 Hrs)

4.1 Essential and trace elements in biological systems, toxic effects of metals (Cd, Hg, Cr, Pb and As), structure and functions of biological membranes, mechanism of ion transport across membranes, sodium pump, ionophores, valinomycin. Phosphate esters in biology, Redox metalloenzymes, cytochromes-cytochrome P450.

4.2 Oxygen carriers and oxygen transport proteins: Structure and functions of haemoglobins and myoglobin, oxygen transport mechanism, cooperativity, Bohr Effect. Structure and functions of haemerythrins and haemocyanin.

4.3 Biochemistry of zinc and copper: Structure and functions of carbonic anhydrase, carboxypeptidase A and superoxide dismutase.

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

- 5.1 Nuclear Reactions: Q value and reaction threshold, reaction cross section, cross section and reaction rate, neutron capture cross section- variation of neutron capture cross section with energy (1/V law). Nuclear fission - fission fragments and mass distribution, fission yields, fission energy, fission cross section and threshold fission neutrons, nuclear fusion reactions and their applications.
- 5.2 Principles of counting technique: G.M. counter, proportional, ionization and scintillation counters, cloud chamber.
- 5.3 Synthesis of transuranic elements: Neptunium, Plutonium, Curium, Berkelium, Einsteinium, Mendelevium, Nobelium, Lawrencium
- 5.4 Analytical applications of radioisotopes-radiometric titrations, kinetics of exchange reactions, measurement of physical constants including diffusion constants, Radioanalysis, Neutron Activation Analysis, Prompt Gama Neutron Activation Analysis and Neutron Absorptiometry.
- 5.5 Radiation chemistry of water and aqueous solutions. Measurement of radiation doses. Relevance of radiation chemistry in biology, organic compounds and radiation polymerization.

**References**

1. J.E. Huheey, E.A. Keiter, R.L. Keiter, *Inorganic Chemistry Principles of Structure and Reactivity*, 4<sup>th</sup> Edn., Harper Collins College Publishers, 1993.
2. F.A. Cotton, G. Wilkinson, C.A. Murillo, M. Bochmann, *Advanced Inorganic Chemistry*, 6<sup>th</sup> edition, Wiley-Interscience, 1999.
3. K.F. Purcell, J.C. Kotz, *Inorganic Chemistry*, Holt-Saunders, 1977.
4. P. Powell, *Principles of Organometallic Chemistry*, 2<sup>nd</sup> Edn., Chapman and Hall, 1988.
5. B.E. Douglas, D.H. McDaniel, J. J. Alexander, *Concepts and Models of Inorganic Chemistry*, 3<sup>rd</sup> Edn. Wiley-India, 2007.
6. B.D. Gupta, A.J Elias, *Basic Organometallic Chemistry*, Universities Press, 2010.
7. R.W. Hay, *Bio-Inorganic Chemistry*, Ellis Horwood, 1984.
8. Sumit Bhaduri, Doble Mukesh, *Homogeneous Catalysis: Mechanism and Industrial Applications*, Wiley Interscience, 2000.
9. Astruc, D.; *Organometallic Chemistry and Catalysis*, Springer Verlag, 2007.
10. Robert H. Crabtree, *The Organometallic Chemistry of the Transition Metals*, 4<sup>th</sup> Edn. Wiley Interscience, 2005.
11. Robert R. Crichton, *Biological Inorganic Chemistry A New Introduction to Molecular Structure and Function*, Elsevier, 2012.
12. H.J. Arnikaar, *Essentials of Nuclear Chemistry*, Wiley Eastern, 1982.
13. S.N. Goshal, *Nuclear Physics*, S. Chand and Company, 2006.

**SEMESTER I****20P1CHET02 : BASIC ORGANIC CHEMISTRY****Credit : 4****Contact Lecture Hours: 72**

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

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

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

- 1.1 Review of basic concepts in organic chemistry: Bonding, hybridisation, MO picture of butadiene and allyl systems.
- 1.2 Electron displacement effects: Inductive effect, electromeric effect, resonance effect, hyperconjugation, steric effect. Bonding weaker than covalent bonds.
- 1.3 Concept of aromaticity: Delocalization of electrons - Hückel's rule, criteria for aromaticity, examples of neutral and charged aromatic systems - annulenes. NMR as a tool, carbon nanotubes and graphene.
- 1.4 Mechanism of electrophilic and nucleophilic aromatic substitution reactions with examples. Arenium ion intermediates.  $S_N1$ ,  $S_NAr$ ,  $S_{RN}1$  and benzyne mechanisms.
- 1.5 Structure and reactions of  $\alpha$ ,  $\beta$ - unsaturated carbonyl compounds involving electrophilic and nucleophilic addition - Michael addition, Mannich reaction, Robinson annulation.

**Unit 2: Physical Organic Chemistry****(9 Hrs)**

- 2.1 Energy profiles. Kinetic versus thermodynamic control of product formation, Hammond postulate, kinetic isotope effects with examples. Linear free energy relationships-Hammett equation, Taft equation.
- 2.2 Catalysis by acids, bases and nucleophiles with examples from acetal and cyanohydrin. Ester formation and hydrolysis reactions of esters -  $A_{AC}2$ ,  $A_{AC}1$ ,  $A_{AL}1$ ,  $B_{AC}2$  and  $B_{AL}1$  mechanisms.

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

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

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

- 4.1 ***Stereoisomerism***: Definition based on symmetry and energy criteria, configuration and conformational stereoisomers, introduction to Akamptisomerism (*basic idea only*)
- 4.2 ***Center of Chirality***: Molecules with C, N, S based chiral centers, absolute configuration, enantiomers, racemic modifications, R and S nomenclature using Cahn-Ingold-Prelog rules, molecules with a chiral center and Cn. molecules with more than one center of chirality, definition of diastereoisomers, constitutionally symmetrical and unsymmetrical chiral molecules, erythro and threo nomenclature.
- 4.3 Axial, planar and helical chirality with examples, stereochemistry and absolute configuration of allenes, biphenyls and binaphthyls, ansa and cyclophanic compounds, spiranes, exo-cyclic alkylidenecycloalkanes.
- 4.4 Topicity and prostereoisomerism, topicity of ligands and faces as well as their nomenclature, NMR distinction of enantiotopic/diastereotopic ligands.
- 4.5 ***Geometrical isomerism***: Nomenclature, E-Z notation, methods of determination of geometrical isomers, interconversion of geometrical isomers.

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

- 5.1 ***Conformational Descriptors*** : Factors affecting conformational stability of molecules, conformational analysis of substituted ethanes, cyclohexane and its derivatives, decalins, adamantane, norbornane, sucrose and lactose.
- 5.2 Conformation and reactivity of elimination (dehalogenation, dehydrohalogenation, semipinacolic deamination and pyrolytic elimination - Saytzeff and Hofmann eliminations), substitution and oxidation of 2° alcohols.
- 5.3 Chemical consequence of conformational equilibrium - Curtin Hammett principle.

**References**

1. D. Hellwinkel, *Systematic nomenclature of organic chemistry*, Springer international Edn.
2. R. Bruckner, *Advanced Organic Chemistry: Reaction Mechanisms*, Academic Press, 2002.
3. F. A. Carey and R. A. Sundberg, *Advanced Organic Chemistry, Part A: Structure and Mechanisms*, Fifth Edition, Springer, New York, 2007.



4. J. Clayden, N. Greeves, S. Warren, P. Wothers, *Organic Chemistry*, Oxford University Press, New York, 2004.
5. Aditi Sangal, *Krishna's Advanced Organic Chemistry*; Volume 1 – Krishna Prakashn Media (P) Ltd.
6. T. H. Lowry and K. S. Richardson, *Mechanism and Theory in Organic Chemistry*, Second Edition, Harper & Row, New York, 1981.
7. N. S. Isaacs, *Physical Organic Chemistry*, ELBS, Longman, UK, 1987.
8. Jack Hine, *Physical Organic Chemistry*, McGraw-Hill; 2<sup>nd</sup> Edition, 1962.
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11. E. L. Eliel and S. H. Wilen, *Stereochemistry of Organic Compounds*, John Wiley & Sons, New York, 1994.
12. N. J. Turro, V. Ramamurthy and J. C. Scaiano, *Principles of Molecular Photochemistry: An Introduction*, University Science books 2009.
13. N.J Turro, *Modern Molecular Photochemistry*, Benjamin Cummings Publishing Company, MenloPark, 1978.
14. K.K.R. Mukherjee, *Fundamentals of Photochemistry*, New Age Publications, New Delhi, 1978.

**SEMESTER I****20P1CHET03 : PHYSICAL CHEMISTRY - I****Credit : 3****Contact Lecture Hours: 54**

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

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

**Unit 1: Classical Thermodynamics****(18 Hrs)**

- 1.1 Mathematical foundations for thermodynamics-variables of thermodynamics, extensive and intensive quantities, equation for total differential, conversion formulas, exact differentials-general formulation, reciprocity characteristics, homogeneous functions, Euler's theorem.(Non-evaluative).
- 1.2 Irreversible processes - Clausius inequality, Free energy, thermodynamic equilibrium, Maxwell relations and significance. Thermodynamic equations of state.
- 1.3 Partial molar quantities, chemical potential and Gibbs-Duhem equation.
- 1.4 Fugacity, relation between fugacity and pressure, Activity and activity coefficient.
- 1.5 Thermodynamics of mixing, Gibbs-Duhem-Margules equation, applications of Gibbs-Duhem-Margules equation- Konovalov's first and second laws, excess thermodynamic functions-free energy, enthalpy, entropy and volume.
- 1.6 Chemical affinity and thermodynamic functions, effect of temperature and pressure on chemical equilibrium.
- 1.7 Third law of thermodynamics, Nernst heat theorem, determination of absolute entropies using third law.
- 1.8 Three component systems-graphical representation. Solid-liquid equilibria, ternary solutions with common ions, hydrate formation, compound formation. Liquid-liquid equilibria-one pair of partially miscible liquids, two pairs of partially miscible liquids, three pairs of partially miscible liquids.

**Unit 2: Kinetic Theory of Gases (9 Hrs)**

- 2.1 Derivation of Maxwell's law of distribution of velocities, graphical representation, experimental verification of the law, most probable velocity, derivation of average, RMS and most probable velocities.
- 2.2 Collision diameter, collision frequency in a single gas and in a mixture of two gases, mean free path, frequency of collision, effusion, the rate of effusion, time dependence of pressure of an effusing gas, the law of corresponding states, transport properties of gases.

**Unit 3: Statistical Thermodynamics (27 Hrs)**

- 3.1 Brief history about the macroscopic and microscopic approach in science, permutation, probability, Stirling's approximation, macrostates and microstates, *equal a priori* principle and thermodynamic probability, thermodynamic probability and entropy, phase-space, ensemble, types of ensembles.
- 3.2 Boltzmann distribution law, partition function and its physical significance, relation between molecular partition function and molar partition function, distinguishable and indistinguishable particles, partition function and thermodynamic functions, separation of partition function-translational, rotational, vibrational, and electronic partition functions, partition function for hydrogen. Thermal de-Broglie wavelength.
- 3.3 Calculation of thermodynamic functions and equilibrium constants, Sackur-Tetrode equation, statistical formulation of third law of thermodynamics, residual entropy, heat capacity of gases - classical and quantum theories.
- 3.4 *Heat capacity of solids*: the vibrational properties of solids, Dulong and Petit's law, Einstein's theory and its limitations, Debye theory and its limitations.
- 3.5 Need for quantum statistics, Bosons and Fermions, *Bose-Einstein statistics*: Bose-Einstein distribution law, Bose-Einstein condensation, first order and higher order phase transitions, liquid helium, *Fermi-Dirac statistics*: Fermi-Dirac distribution law, application in electron gas, thermionic emission.
- Comparison of three statistics.

**References**

1. Irving M. Klotz, Robert M. Rosenberg, *Chemical Thermodynamics*, John Wiley & Sons, INC Publication, 2008.
2. R.P. Rastogi, R.R. Misra, *An introduction to Chemical Thermodynamics*, Vikas publishing house, 1996.
3. J. Rajaram, J.C. Kuriakose, *Thermodynamics*, S Chand and Co., 1999.
4. M.W. Zemansky, R.H. Dittman, *Heat and Thermodynamics*, Tata McGraw Hill, 1981.
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10. J. Kestin, J.R. Dorfman, *A Course in Statistical Thermodynamics*, Academic Press, 1971.
11. M.C. Gupta, *Statistical Thermodynamics*, New age international, 2007.

## SEMESTER I

## 20P1CHET04 : QUANTUM CHEMISTRY AND GROUP THEORY

Credit: 4

Contact Lecture Hours: 72

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

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

- 1.1 Symmetry elements and symmetry operations.
- 1.2 Determination of point groups of molecules and ions (organic / inorganic / complex) belonging to  $C_n$ ,  $C_s$ ,  $C_i$ ,  $C_{nv}$ ,  $C_{nh}$ ,  $C_{\infty v}$ ,  $D_{nh}$ ,  $D_{\infty h}$ ,  $D_{nd}$ ,  $T_d$  and  $O_h$  point groups.
- 1.3 Symmetry in crystals: 32 crystallographic point groups (*no derivation*), Hermann-Mauguin symbols. Screw axis-pitch and fold of screw axis, glide planes, space groups (*elementary idea only*)
- 1.4 Mathematical groups: Properties, Abelian groups, cyclic groups, sub groups, similarity transformation, classes –  $C_{2v}$ ,  $C_{3v}$  and  $C_{2h}$ .
- 1.5 Group multiplication tables (GMTs) –  $C_{2v}$ ,  $C_{3v}$  and  $C_{2h}$ , isomorphic groups.
- 1.6 Matrix representation of elements like E,  $C_n$ ,  $S_n$ , I,  $\sigma$ -matrix representation of point groups like  $C_{2v}$ ,  $C_{3v}$ ,  $C_{2h}$ ,  $C_{4v}$  – trace /character, block factored matrices.
- 1.7 Reducible and irreducible representations, standard reduction formula, statement of great orthogonality theorem (GOT). Construction of character tables for  $C_{2v}$ ,  $C_{2h}$ ,  $C_{3v}$  and  $C_{4v}$ .
- 1.8 Application in chemical bonding: Projection operator, transformation properties of atomic orbitals, construction of symmetry adapted linear combination of atomic orbitals (SALCs) of  $C_{2v}$ ,  $C_{3v}$ ,  $D_{3h}$  and  $C_{2h}$  molecules.

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

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

2.2. Postulates of Quantum Mechanics.

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

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

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

*Expectation value postulate.*

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

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

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

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

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

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

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

**References**

1. I.N. Levine, *Quantum Chemistry*, 7<sup>th</sup> Edn., Pearson Education Inc., 2016.
2. P.W. Atkins, R.S. Friedman, *Molecular Quantum Mechanics*, 4<sup>th</sup> Edn., Oxford University Press, 2005.
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## SEMESTER II

## 20P2CHET05 : INORGANIC CHEMISTRY - II

Credit : 4

Contact Lecture Hours: 72

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

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

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

- 1.1 Classification of complexes based on coordination numbers and possible geometries, sigma and pi bonding ligands such as CO, NO, CN<sup>-</sup>, R<sub>3</sub>P, and Ar<sub>3</sub>P. Stability of complexes, thermodynamic aspects of complex formation-Irving William order of stability, chelate effect.
- 1.2 Splitting of d orbitals in octahedral, tetrahedral, square planar, square pyramidal and trigonal bipyramidal fields, LFSE, Dq values, Jahn Teller (JT) effect, theoretical failure of crystal field theory, evidence of covalency in the metal-ligand bond, nephelauxetic effect, ligand field theory, molecular orbital theory - M.O energy level diagrams for octahedral and tetrahedral complexes without and with  $\pi$  - bonding, experimental evidences for pi-bonding.

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

- 2.1 Electronic Spectra of complexes: Term symbols of d<sup>n</sup> system, Racah parameters, splitting of terms in weak and strong octahedral and tetrahedral fields, correlation diagrams for d<sup>1</sup> and d<sup>9</sup> ions in octahedral and tetrahedral fields (*qualitative approach*), d-d transitions, selection rules for electronic transitions-effect of spin orbit coupling and vibronic coupling.
- 2.2 Interpretation of electronic spectra of complexes: Orgel diagrams and demerits, Tanabe Sugano diagrams, calculation of Dq, B and  $\beta$  (*Nephelauxetic ratio*) values, spectra of complexes with lower symmetries, charge transfer spectra, luminescence spectra.
- 2.3 Magnetic properties of complexes-paramagnetic and diamagnetic complexes, molar susceptibility, Gouy method for the determination of magnetic moment of complexes, spin only magnetic moment. Temperature dependence of magnetism- Curie's law, Curie-Weiss law,



temperature independent paramagnetism (TIP), spin state cross over, antiferromagnetism-inter and intra molecular interaction, anomalous magnetic moments.

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

- 3.1 Thermodynamic and kinetic stability, kinetics and mechanism of nucleophilic substitution reactions in square planar complexes- trans effect-theory and applications, effect of entering ligand, effect of leaving group and effect of ligands already present on reaction rate, effect of solvent and reaction pathways, substitution in tetrahedral and five-coordinate complexes.
- 3.2 Kinetics and mechanism of octahedral substitution- water exchange, dissociative and associative mechanisms, base hydrolysis, racemization reactions, solvolytic reactions (acidic and basic). Replacement reactions involving multidentate ligands - formation of chelates, effect of  $H^+$  on the rates of substitution of chelate complexes, metal ion assisted and ligand assisted dechelation.
- 3.3 Electron transfer reactions: Outer sphere mechanism-Marcus theory, inner sphere mechanism-Taube mechanism, mixed outer and inner sphere reactions, two electron transfer and intramolecular electron transfer.

**Unit 4: Stereochemistry of Coordination Compounds (9 Hrs)**

- 4.1 Geometrical and optical isomerism in octahedral complexes, resolution of optically active complexes, determination of absolute configuration of complexes by ORD and circular dichroism, stereoselectivity and conformation of chelate rings, asymmetric synthesis catalyzed by coordination compounds,
- 4.2 Linkage isomerism: Electronic and steric factors affecting linkage isomerism, symbiosis-hard and soft ligands, Prussian blue and related structures, Macrocycles crown ethers.

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

- 5.1 Term symbols for lanthanide ions, inorganic compounds and coordination complexes of the lanthanoids upto coordination No.12, electronic spectra and magnetic properties of lanthanoid complexes, organometallic complexes of the lanthanoids -  $\sigma$ -bonded complexes, cyclopentadienyl complexes, organolanthanoid complexes as catalysts.
- 5.2 General characteristics of actinoids-difference between 4f and 5f orbitals, coordination complexes of the actinoids- sandwich complexes, coordination complexes and organometallic compounds of thorium and uranium, comparative account of coordination chemistry of lanthanoids and actinoids with special reference to electronic spectra and magnetic properties.

**References**

1. F.A. Cotton, G. Wilkinson, *Advanced Inorganic Chemistry: A Comprehensive Text*, 3<sup>rd</sup> Edn., Interscience, 1972. PROGRAM STRUCTURE
2. J.E. Huheey, E.A. Keiter, R.A. Keiter, *Inorganic Chemistry Principles of Structure and Reactivity*, 4<sup>th</sup> Edn., Pearson Education India, 2006.

3. K.F. Purcell, J.C. Kotz, *Inorganic Chemistry*, Holt-Saunders, 1977.
4. F. Basolo, R.G. Pearson, *Mechanisms of Inorganic Reaction*, John Wiley & Sons, 2006.
5. B.E. Douglas, D.H. McDaniel, J.J. Alexander, *Concepts and Models of Inorganic Chemistry*, 3<sup>rd</sup> Edn., Wiley-India, 2007.
6. R.S. Drago, *Physical Methods in Chemistry*, Saunders College, 1992.
7. B.N. Figgis, M.A. Hitchman, *Ligand Field Theory and its Applications*, Wiley-India, 2010.
8. J.D. Lee, *Concise Inorganic Chemistry*, 4<sup>th</sup> Edn., Wiley-India, 2008
9. R. G. Wilkins, *Kinetics and Mechanisms of Reactions of Transition Metal Complexes*, Wiley VCH, 2002.
10. G. A. Lawrance, *Introduction to Coordination Chemistry*, John Wiley & Sons Ltd, 2010.
11. C. E. Housecroft, A. G. Sharpe, *Inorganic Chemistry*, Pearson, 2012.

## SEMESTER II

## 20P2CHET06 : ORGANIC REACTION MECHANISM

Credit : 4

Contact Lecture Hours : 72

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

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

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

- 1.1 Review of organic reaction mechanisms with special reference to nucleophilic and electrophilic substitution at aliphatic carbon ( $S_N^1$ ,  $S_N^2$ ,  $S_Ni$ ,  $SE_1$  and  $SE_2$ ) elimination ( $E_1$  and  $E_2$ ) and addition reactions (Regioselectivity: Markovnikov's addition - carbocation mechanism, anti-Markovnikov's addition - radical mechanism). Elimination *vs* Substitution.
- 1.2 A comprehensive study on the effect of substrate, reagent, leaving group, solvent, ambident nucleophile and neighbouring group on nucleophilic substitution ( $S_N1$  and  $S_N2$ ) and elimination ( $E_1$  and  $E_2$ ) reactions.
- 1.3 Electrophilic substitution *via* enolization and Stork-enamine reaction. Von Ritter, Vilsmeier formylation, Jacobson and Gatterman-Koch reactions.

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

- 2.1 Formation, structure and stability of carbanions. Reactions of carbanions: C-X bond (X = C, O, N) formations through the intermediary of carbanions. Chemistry of enolates and enamines. Kinetic and Thermodynamic enolates-lithium and boron enolates in aldol Alkylation and acylation of enolates.
- 2.2 Nucleophilic additions to carbonyls groups. Name reactions under carbanion chemistry – Mechanism of Claisen, Dieckmann, Knoevenagel, Stobbe, Darzen and acyloin condensations, Shapiro reaction and Julia elimination. Favorski rearrangement.

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

### Unit 3: Chemistry of Carbocations (9Hrs.)

- 3.1 Formation, structure and stability of carbocations. Classical and non-classical carbocations.
- 3.2 C-X bond (X = C, O, N) formations through the intermediary of carbocations. Molecular rearrangements including Wagner-Meerwein, Pinacol-pinacolone, semi-pinacol, Dienone-phenol and Benzilic acid rearrangements, Noyori annulation, Prins reaction.
- 3.3 C-C bond formation involving carbocations: Oxymercuration, halolactonisation.

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

- 4.1 Structure of carbenes (singlet and triplet) - generation of carbenes - addition and insertion reactions.
- 4.2 Rearrangement reactions of carbenes such as Wolff rearrangement - generation and reactions of ylids by carbenoid decomposition.
- 4.3 Structure, generation and reactions of nitrene and related electron deficient nitrene intermediates.
- 4.4 Hoffmann, Curtius, Lossen, Schmidt and Beckmann rearrangement reactions.
- 4.5 Arynes: Generation, structure, stability and reactions. Orientation effect- amination of haloarenes.

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

- 5.1 Generation of radical intermediates and its (a) addition to alkenes, alkynes (inter & intramolecular) for C-C bond formation - Baldwin's rules (b) fragmentation and rearrangements – Hydroperoxide: formation, rearrangement and reactions. Auto-oxidation.
- 5.2 Named reactions involving radical intermediates: Barton deoxygenation and decarboxylation, McMurry coupling.

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

- 6.1 Classification: Electrocyclic, sigmatropic, cycloaddition, chelotropic and ene reactions. Woodward Hoffmann rules - frontier orbital and orbital symmetry correlation approaches - PMO method (*for electrocyclic and cycloaddition reactions only*)
- 6.2 Highlighting pericyclic reactions in organic synthesis such as Claisen, Cope, Wittig, Mislow-Evans and Sommelet-Hauser rearrangements. Diels-Alder and Ene reactions (*with stereochemical aspects*), dipolar cycloaddition (*introductory*).

- 6.3 Unimolecular pyrolytic elimination reactions: cheletropic elimination, decomposition of cyclic azo compounds,  $\beta$ -eliminations involving cyclic transition states such as N-oxides (Cope reaction), acetates and xanthates (Chugayev reaction)
- 6.4 Introduction to Click reactions - Mechanism of the Huisgen Azide - Alkyne 1, 3-Dipolar Cycloaddition, Staudinger ligation and Staudinger reduction.

## References

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

## SEMESTER II

### 20P2CHET07 : PHYSICAL CHEMISTRY - II

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

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

	<i>Course Outcome</i>	<i>POs / PSOs</i>	<i>CL</i>	<i>KC</i>	<i>Class Sessions</i>
<b>CO1</b>	Analyze atomic, molecular and spin resonance spectroscopy.	PO 1 PSO 2	AN	F	12
<b>CO2</b>	Define aspects of specific spectroscopic techniques, applications of molecular symmetry in spectroscopy.	PO 1 PSO 1	U	C	27
<b>CO3</b>	Understand the fundamental concepts of light-matter interaction, lasers and laser systems, detectors and other relevant aspects of instrumentation necessary for spectroscopy and imaging.	PO 1 PSO 1	U	F	9
<b>CO4</b>	Ability to understand theory and application to mass spectrometry, ultraviolet and visible spectroscopy, infrared spectroscopy, Raman, fluorescence, nuclear magnetic resonance spectroscopy.	PO 1 PSO 2	U	C	24

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

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

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

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

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

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

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

3.2 Vibrational spectra of polyatomic molecules, normal modes of vibrations, combination and

difference bands, Fermi resonance. FT technique, introduction to FTIR spectroscopy. Instrumentation of FTIR.

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

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

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

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

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

5.1 Theory of NMR Spectroscopy: Interaction between nuclear spin and applied magnetic field, important magnetically active nuclei. Nuclear energy levels, population of energy levels, Larmor precession, relaxation methods. Chemical shift and its representation-  $\delta$  scale of PMR and CMR. Spin-spin coupling: Theory and illustration with AX system.

5.2 Fourier Transformation (FT) NMR Spectroscopy: Instrumentation of NMR technique, magnets, probe and probe tuning, Creating NMR signals, effect of pulses, rotating frame reference, FID, FT technique, data acquisition and storage. Pulse sequences- Pulse width, spins and magnetisation vector.

5.3 Solid state NMR-Applications. Magic Angle Spinning (MAS).

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

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

6.2 Theory and important applications of NQR Spectroscopy.

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

#### **References**

1. C.N. Banwell, E.M. McCash, *Fundamentals of Molecular Spectroscopy*, 4<sup>th</sup> Edn., Tata McGraw Hill, 1994.

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

## SEMESTER II

### 20P2CHET08 : THEORETICAL AND COMPUTATIONAL CHEMISTRY

**Credit: 3**

**Contact Lecture Hours: 72**



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

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

### Unit 1: Application of Group Theory in Spectroscopy

(18 Hrs)

- 1.1. Vibrational mode analysis using group theory taking H<sub>2</sub>O, NH<sub>3</sub> and *trans*-N<sub>2</sub>F<sub>2</sub> as examples using symmetry coordinates and internal coordinates method, prediction of IR and Raman activity, rule of mutual exclusion, redundant modes, out of plane modes.
- 1.2. Application in uv-visible spectroscopy, selection rules, orbital selection rules, transitions between non-degenerate states, prediction of electronic transitions in C<sub>2v</sub>, C<sub>3v</sub>, C<sub>4v</sub>, C<sub>2h</sub> and C<sub>4h</sub> using direct product terms, spin selection rules, relaxation in selection rules and distortion .
- 1.3. Application in hybridization, determination of hybridization and hybrid functions in CH<sub>4</sub>, BF<sub>3</sub> and PCl<sub>5</sub>
- 1.4. Group theory and optical activity (*brief study*)

### Unit 2 : Approximation Methods in Quantum Mechanics

(18 Hrs)

- 2.1 Many-body problem and the need of approximation methods, independent particle model. Variation method: Variation theorem with proof, illustration of variation theorem using the trial function  $\psi(x) = x(a-x)$  for particle in a 1D-box and using the trial function  $e^{-\alpha r}$  for the hydrogen atom, variation treatment for the ground state of helium atom.
- 2.2 Perturbation method, time-independent perturbation method (*non-degenerate case only*), first order correction to energy and wave function, illustration by application to particle in a 1D-box with slanted bottom, perturbation treatment of the ground state of the helium atom. Qualitative idea of Hellmann-Feynman theorem.
- 2.3 Hartree-Fock method, multi-electron atoms. Hartree-Fock equations (*no derivation*). The Fock operator, core hamiltonian, coulomb operator and exchange operator. Qualitative treatment of Hartree-Fock Self-Consistent Field (HFSCF) method. Roothan's concept of basis functions, Slater type orbitals (STO) and Gaussian type orbitals (GTO), sketches of STO and GTO.

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

- 3.1 Schrödinger equation for molecules. Born-Oppenheimer approximation, valence bond (VB) theory, VB theory of H<sub>2</sub> molecule, singlet and triplet state functions (spin orbitals) of H<sub>2</sub>.
- 3.2 Molecular Orbital (MO) theory, MO theory of H<sub>2</sub><sup>+</sup> ion, MO theory of H<sub>2</sub> molecule, MO treatment of homonuclear diatomic molecules Li<sub>2</sub>, Be<sub>2</sub>, N<sub>2</sub>, O<sub>2</sub> and F<sub>2</sub> and hetero nuclear diatomic molecules LiH, CO, NO and HF, bond order. Correlation diagrams, non-crossing rule, spectroscopic term symbols for diatomic molecules, comparison of MO and VB theories.
- 3.3 Hybridization, quantum mechanical treatment of sp, sp<sup>2</sup> and sp<sup>3</sup> hybridisation. Semiempirical MO treatment of planar conjugated molecules, Hückel Molecular Orbital (HMO) theory of ethene, allyl systems, butadiene and benzene. Calculation of charge distributions, bond orders and free valency.

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

- 4.1 Introduction and scope of computational chemistry, potential energy surface, conformational search, global minimum, local minima, saddle points.
- 4.2 *Ab-initio methods*: A review of Hartree-Fock method, self-consistent field (SCF) procedure. Roothaan concept basis functions. Basis sets and its classification: Slater type and Gaussian type basis sets, minimal basis set, Pople style basis sets. Hartree-Fock limit. Post Hartree-Fock methods - introduction to Møller-Plesset perturbation theory, configuration interaction, coupled cluster and semi empirical methods.
- 4.3 *Introduction to Density Functional Theory (DFT) methods*: Hohenberg-Kohn theorems, Kohn-Sham orbitals, exchange correlation functional, local density approximation, generalized gradient approximation, hybrid functionals (*only the basic principles and terms need to be introduced*).
- 4.4 Comparison of ab-initio, semi empirical and DFT methods.
- 4.5 *Molecular geometry input*: Cartesian coordinates and internal coordinates, Z-matrix, Z-matrix of single atom, diatomic molecule, non-linear triatomic molecule, linear triatomic molecule, polyatomic molecules like ammonia, methane and ethane. General format of GAMESS / Firefly input file, single point energy calculation, geometry optimization, constrained optimization and frequency calculation. Koopmans' theorem.
- 4.6 Features of molecular mechanics force field-bond stretching, angle bending, torsional terms, non-bonded interactions and electrostatic interactions. Commonly used force fields- AMBER and CHARMM.

**References**

1. N. Levine, *Quantum Chemistry*, 7<sup>th</sup> Edn., Pearson Education Inc., 2016.
2. P.W. Atkins, R.S. Friedman, *Molecular Quantum Mechanics*, 4<sup>th</sup> Edn., Oxford University Press, 2005.

3. D.A. McQuarrie, *Quantum Chemistry*, University Science Books, 2008.
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10. M.S. Pathania, *Quantum Chemistry and Spectroscopy (Problems & Solutions)*, Vishal Publications, 1984.
11. F.A. Cotton, *Chemical Applications of Group Theory*, 3<sup>rd</sup> Edn., Wiley Eastern, 1990.
12. L. H. Hall, *Group Theory and Symmetry in Chemistry*, McGraw Hill, 1969.
13. V. Ramakrishnan, M.S. Gopinathan, *Group Theory in Chemistry*, Vishal Publications, 1992.
14. S. Swarnalakshmi, T. Saroja, R.M. Ezhilarasi, *A Simple Approach to Group Theory in Chemistry*, Universities Press, 2008.
15. S.F.A. Kettle, *Symmetry and Structure: Readable Group Theory for Chemists*, 3<sup>rd</sup> Edn., Wiley, 2007.
16. A. Vincent, *Molecular Symmetry and Group Theory: A Programmed Introduction to Chemical Applications*, 2<sup>nd</sup> Edn., Wiley, 2000.
17. A.S. Kunju, G. Krishnan, *Group Theory and its Applications in Chemistry*, PHI Learning, 2010.
18. K.I. Ramachandran, G. Deepa, K. Namboori, *Computational Chemistry and Molecular Modeling: Principles and Applications*, Springer, 2008.
19. A. Hinchliffe, *Molecular Modelling for Beginners*, 2<sup>nd</sup> Edn., John Wiley & Sons, 2008.
20. C.J. Cramer, *Essentials of Computational Chemistry: Theories and Models*, 2<sup>nd</sup> Edn., John Wiley & Sons, 2004.
21. D.C. Young, *Computational Chemistry: A Practical Guide for Applying Techniques to Real World Problems*, John Wiley & Sons, 2001.

**Softwares:**

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

B) Ab initio, semiempirical and DFT:

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

C) Graphical User Interface (GUI):

1. Gabedit available from <http://gabedit.sourceforge.net/>

2. wxMacMolPlt available from <http://www.scl.ameslab.gov/MacMolPlt>

### SEMESTERS I & II

#### 20P2CHEP01 : INORGANIC CHEMISTRY PRACTICAL-I

**Credit: 3**

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

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

	<i>Course Outcome</i>	<i>POs / PSOs</i>	<i>CL</i>	<i>KC</i>	<i>Class Sessions</i>
<b>CO1</b>	Illustrate the separation and identification of mixture of cations.	PO 1 PSO 5	A	P	54
<b>CO2</b>	Perform colorimetric estimations.	PO 1 PSO 5	A	P	27

CO3	Prepare and characterize coordination compounds.	PO 1 PSO 5	A	P	27
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## PART I

Separation and identification of a mixture of four cations (a mixture of two familiar ions such as  $\text{Ag}^+$ ,  $\text{Hg}^{2+}$ ,  $\text{Pb}^{2+}$ ,  $\text{Cu}^{2+}$ ,  $\text{Bi}^{2+}$ ,  $\text{Cd}^{2+}$ ,  $\text{As}^{3+}$ ,  $\text{Sn}^{2+}$ ,  $\text{Sb}^{3+}$ ,  $\text{Fe}^{2+}$ ,  $\text{Fe}^{3+}$ ,  $\text{Al}^{3+}$ ,  $\text{Cr}^{3+}$ ,  $\text{Zn}^{2+}$ ,  $\text{Mn}^{2+}$ ,  $\text{Co}^{2+}$ ,  $\text{Ni}^{2+}$ ,  $\text{Ca}^{2+}$ ,  $\text{Sr}^{2+}$ ,  $\text{Ba}^{2+}$ ,  $\text{Mg}^{2+}$ ,  $\text{Li}^+$ ,  $\text{Na}^+$ ,  $\text{K}^+$  and  $\text{NH}_4^+$  and two less familiar metal ions such as Tl, W, Se, Mo, Ce, Th, Ti, Zr, V, U and Li).

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

## PART II

Colorimetric estimation of Fe, Cu, Ni, Mn, Cr, and  $\text{NH}_4^+$ , nitrate and phosphate ions.

## PART III

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

- Tris (thiourea)copper(I) complex
- Potassium tris (oxalate) aluminate (III).
- Hexammine cobalt (III) chloride.
- Tetrammine copper (II) sulphate.
- Schiff base complexes of various divalent metal ions.
- Bis(dimethylglyoximato)nickel(II)
- Prussian blue

## References

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

**SEMESTERS I & II****20P2CHEP02 : ORGANIC CHEMISTRY PRACTICAL - I****CREDIT: 3****Contact Lab Hours: 54+54=108**

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

	<i>Course Outcome</i>	<i>POs / PSOs</i>	<i>CL</i>	<i>KC</i>	<i>Class Sessions</i>
<b>CO1</b>	Carry out different methods of separation and purification of organic compounds.	PO 1 PSO 5	A	P	54
<b>CO2</b>	Apply the methods of separation and purification to organic binary mixtures.	PO 1	A	P	27

		PSO 5			
CO3	Construct the organic structures and reaction schemes using ChemSketch.	PO 1 PSO 5	A	P	27

### PART I

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

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

### PART II

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

### PART III

Drawing the structures of organic molecules and reaction schemes by Chems sketch.

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

### References

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

**SEMESTERS I & II****20P2CHEP03 : PHYSICAL CHEMISTRY PRACTICAL-I****Credit: 3****Contact Lab Hours: 72+72 =144**

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

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

	<i>Course Outcome</i>	<i>POs / PSOs</i>	<i>CL</i>	<i>KC</i>	<i>Class Sessions</i>



<b>CO1</b>	Illustrate experiments related to adsorption, phase diagrams, distribution law and surface tension.	PO 1 PSO 5	A	P	100
<b>CO2</b>	Apply the methods of computational chemistry to solve different problems of chemistry.	PO 1 PSO 5	A	P	44

## **Part A**

### **I. Adsorption**

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

### **II. Phase diagrams**

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

### **III. Distribution law**

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

### **IV. Surface tension**

1. Determination of the surface tension of a liquid by:
  - a) Drop number method
  - b) Drop weight method
2. Determination of the composition of two liquids by surface tension measurements
3. To determine the critical Micelle concentration of sodium lauryl sulphate
4. Determine the surface excess of amyl alcohol.

### **References**

01. J.B. Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, 2001.
02. G.W. Garland, J.W. Nibler, D.P. Shoemaker, Experiments in Physical Chemistry, 8<sup>th</sup> Edn. McGraw Hill, 2009.
03. B. Viswanathan, Practical Physical chemistry, Viva Pub., 2005
04. Saroj Kumar and Naba Kumar, Physical Chemistry Practical, New Central Book Agency, 2012.

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

## **Part B**

### **List of Computational Chemistry Experiments (Second Module of Physical Chemistry Practical -I)**

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

1. Geometry optimization and single point energy calculations of simple organic molecules
2. Calculation of energy gap between HOMO and LUMO in simple molecules and visualization of molecular orbitals
3. Calculation of dipole moment in polar organic molecules.
4. Calculation of electrostatic charges of atoms in organic molecules using population analysis
5. Calculation of Resonance energy of aromatic compounds
6. Prediction of the stability of *ortho*, *meta*, *para* products of nitration of aromatic ring using computational chemistry calculations.
7. Calculation of IR stretching frequencies of groups and visualization of normal modes of vibration in organic molecules.
8. Calculation of dimerization energy of carboxylic acids
9. Perform the conformational analysis of butane using potential energy scan
10. Find the transition state of simple organic reactions and plot the reaction profile.
11. Determination of heat of hydration of organic molecules.
12. Find the Gibbs free energy of simple gaseous phase reactions and calculate equilibrium constant.
13. Spectral analysis (UV, IR and NMR) of simple organic molecules.
14. Perform molecular dynamic simulations of smaller molecules in water.
15. Calculation of pK<sub>a</sub> of simple organic molecules and compare it with experimental values
16. Docking studies involving protein ligand interactions.
17. Calculation of electrophilicity index in hard-soft acids and bases.

### **Reference**

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

**SEMESTER III****20P3CHET09 : INORGANIC CHEMISTRY - III****Credit: 4****Contact Lecture Hours: 72**

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

	<i>Course Outcome</i>	<i>POs / PSOs</i>	<i>CL</i>	<i>KC</i>	<i>Class Sessions</i>
<b>CO1</b>	Describe the structure, reactions and phase transitions of solid state	PO 1 PSO 1	U	F	18
<b>CO2</b>	Explain the electrical, magnetic and optical properties of solids.	PO 1 PSO 1	R	F	18

<b>CO3</b>	Explain the structure and applications of inorganic chains, rings, cages and clusters, and organometallic polymers.	PO 1 PSO 3	A	C	27
<b>CO4</b>	Describe the synthesis of solids and applications of magnetonano particles.	PO 1 PSO 3	U	C	9

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

- 1.1 Structure of solids: Imperfections in solids- line defects and plane defects. Structure of the following compounds - Zinc blende, Wurtzite, Rutile, fluorite, antiferite, Nickel Arsenide, Perovskite and Ilmenite. Spinel, inverse spinel structures.
- 1.2 Solid state reactions, diffusion coefficient, mechanisms, vacancy diffusion. Thermal decomposition of solid: Type I reactions, Type II reactions.
- 1.3 Phase transition in solids: Classification of phase transitions, first and second order phase transitions, martensitic transformations, order-disorder transitions and spinodal decomposition, kinetics of phase transitions, sintering, growing single crystals-crystal growth from solution, growth from melt and vapour deposition technique.

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

- 2.1 Free electron theory of solids. Band theory of solids: Applications to Transition metal compounds and compounds like NaCl, MgO and fullerenes. Energy bands-conductors and non-conductors, Mechanism of intrinsic and extrinsic semiconductors. Mobility of charge carriers-Hall Effect (derivation required). Piezo electricity, pyroelectricity and ferro electricity-hysteresis.
- 2.2 Magnetic properties of transition metal oxides, garnets, spinels, ilmenites and perovskites, magnetoplumbites. Photoconductivity, photovoltaic effects, luminescence, applications of optical properties-phosphors, solid state lasers and solar cells.
- 2.3 Conductivity of pure metals. Super conductivity-Type I and Type II superconductors, Meisner effect, BCS theory of superconductivity (derivation not required)-Cooper pairs. High temperature superconductors, super conducting cuprates - YBaCu oxide system. Josephson's Junction, conventional superconductors, organic superconductors, fullerenes, carbon nanotubes and graphenes.

**Unit 3: Inorganic Chains and Rings****(9 Hrs)**

- 3.1 *Chains*: Catenation, heterocatenation, silicones. Zeolites: Synthesis, structure and applications, isopoly acids of vanadium, molybdenum and tungsten, heteropoly acids of Mo and W, polythiazil-one dimensional conductors. Infinite metal chains.

- 3.2 *Rings*: Topological approach to boron hydrides, styx numbers. Heterocyclic inorganic ring systems: Structure and bonding in phosphorous-sulphur and sulphur-nitrogen compounds. Homocyclic inorganic ring systems: Structure and bonding in sulphur, selenium and phosphorous compounds.

#### Unit 4: Inorganic Cages and Clusters

(9 Hrs)

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

#### Unit 5: Organometallic Polymers

(9 Hrs)

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

#### Unit 6: Synthesis of Solids and Magnetic Nanoparticles

(9 Hrs)

- 6.1 *Synthesis of Solids*: Nucleation, growth, epitaxy and topotaxy, methods for the synthesis of  $MgAl_2O_4$ , silica glass, indium tin oxide and their coatings, zeolites and alumina based abrasives, hydrothermal synthesis, intercalation and deintercalation, preparation of thin films, electrochemical methods, chemical vapour deposition. Synthesis of amorphous silica and diamond films, sputtering and laser ablation.
- 6.2 Magnetic nanoparticles, superparamagnetism and thin films, applications of magnetic nanoparticles - data storage, Magnetic Resonance Imaging (MRI) and Contrast Enhancement using magnetic nanoparticles, biomedical applications of magnetic nanoparticles.

#### References

1. L.V. Azaroff, *Introduction to Solids*, Mc Graw Hill, 1984.
2. A.R. West, *Solid State Chemistry and its Applications*, Wiley-India, 2007.
3. D.K. Chakrabarty, *Solid State Chemistry*, New Age Pub., 2010.
4. D.M. Adams, *Inorganic Solids: An Introduction to Concepts in Solid State Structural Chemistry*, Wiley, 1974.
5. C.N.R. Rao, K.J. Rao, *Phase Transitions in Solids*, McGraw Hill, 2010.
6. B.E. Douglas, D.H. McDaniel, J.J. Alexander, *Concepts and Models of Inorganic Chemistry*, 3<sup>rd</sup> Edn., John Wiley & sons, 2006.
7. A. Earnshaw, *Introduction to Magnetochemistry*, Academic Press, 1968.

8. J.E. Huheey, E.A. Keiter, R.L. Keiter, *Inorganic Chemistry Principles of Structure and Reactivity*, 4<sup>th</sup> Edn., Harper Collins College Pub., 1993.
9. F.A. Cotton, G. Wilkinson, C.A. Murillo, M. Bochmann, *Advanced Inorganic Chemistry*, 6<sup>th</sup> Edn., Wiley-Interscience, 1999.
10. K.F. Purcell, J.C. Kotz, *Inorganic Chemistry*, Holt-Saunders, 1977.
11. Wai Kee Li, Gong-Du Zhou, Thomas Chung Wai Mak, *Advanced Structural Inorganic Chemistry*, International Union of Crystallography, 2008.
12. Matthias Driess, Heinrich Nöth, *Molecular Clusters of the Main Group Elements*, Wiley-VCH, 2004.
13. Richard J.D. Tilley, *Understanding Solids*, 2<sup>nd</sup> edition, Wiley, 2013.
14. G.L. Hornyak, J.J. Moore, H.F. Tibbals, J. Dutta, *Fundamentals of Nanotechnology*, CRC Press, 2009.
15. Chris Binns, *Introduction to Nanoscience and Nanotechnology*, Wiley, 2010.
16. Vadapalli Chandrasekhar, *Inorganic and Organometallic Polymers*, Springer, 2005.
17. Anthony R. West, *Basic Solid State Chemistry*, John Wiley and Sons, 1988.

### SEMESTER III

#### 20P3CHET10 : ORGANIC SYNTHESSES

**Credit: 4**

**Contact Lecture Hours: 72**

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

	<i>Course Outcome</i>	<i>POs / PSOs</i>	<i>CL</i>	<i>KC</i>	<i>Class Sessions</i>
<b>CO1</b>	Describe the applications of oxidation and reduction techniques in organic syntheses.	PO 1 PSO 2	A	C	18
<b>CO2</b>	Illustrate modern synthetic methods and applications of reagents.	PO 1 PSO 1	U	C	15

<b>CO3</b>	Explain different methods for the construction of carbocyclic and heterocyclic ring systems.	PO 1 PSO 3	U	F	12
<b>CO4</b>	Understand the principles and applications of protecting groups in chemistry.	PO 1 PSO 3	U	C	9
<b>CO5</b>	Apply retrosynthetic analysis to design the synthesis of a target molecule.	PO 1 PSO 3	U	C	9

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

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

1.2 (a) Catalytic hydrogenation (Heterogeneous: Palladium/Platinum/Rhodium and Nickel. Homogeneous: Wilkinson).(b) Metal based reductions- Birch reduction, pinacol formation, acyloin formation (c) Hydride transfer reagents from Group III and Group IV in reductions - LiAlH<sub>4</sub>, DIBAL-H, Red-Al, NaBH<sub>4</sub> and NaCNBH<sub>3</sub>, Selectrides,trialkylsilanes and trialkylstannane, Meerwein-Pondorff-Verleyreducxtion, Baker's yeast.

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

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

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

**Unit 3: Construction of Carbocyclic and Heterocyclic Ring Systems****(12 Hrs)**

- 3.1 The synthesis of four, five and six-membered rings- ketene cycloaddition (inter- and intramolecular)- Pauson-Khand reaction, Volhardt reaction, Bergman cyclization, Nazarov cyclization, radical cyclization, Robinson annulation.
- 3.2 Inter-conversion of ring systems (contraction and expansion)-Demjenov reaction, Construction of macrocyclic rings - ring closing metathesis.
- 3.3 Formation of heterocyclic rings: Preparation and structure of the following heterocyclics- azeridine, oxirane, thirane, oxaziridine, azetidine and thietane, 5-membered ring heterocyclic compounds with one or more than 1 hetero atom like N, S or O- Pyrrole, furan, thiophene, imidazole, thiazole and oxazole.

**Unit 4: Protecting Group Chemistry****(9 Hrs)**

- 4.1 Protection and deprotection of hydroxy, carboxyl, carbonyl, and amino groups. Chemo- and regioselective protection and deprotection. Illustration of protection and deprotection in synthesis.
- 4.2 Protection and deprotection in peptide synthesis: Common protecting groups used in peptide synthesis- Protecting groups used in solution phase and solid phase peptide synthesis (SPPS).
- 4.3 Role of trialkyl silyl group in organic synthesis.

**Unit 5: Retrosynthetic Analysis****(9 Hrs)**

- 5.1 Basic principles and terminology of retrosynthesis: synthesis of aromatic compounds, one group and two group C-X disconnections; one group C-C and two group C-C disconnections.
- 5.2 Amine and alkene synthesis: important strategies of retrosynthesis, functional group transposition, important functional group interconversions. Retrosynthesis of luciferin. Functional equivalents and reactivity - Umpolung reaction (*Ireland-Claisen rearrangement*).

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

- 6.1 Concept of molecular recognition- host-guest complex formation- Forces involved in molecular recognition.
- 6.2 Molecular receptors: Cyclodextrins, crown ethers, cryptands, spherands, tweezers, carcerands, cyclophanes, calixarenes.
- 6.3 Importance of molecular recognition in nucleic acids and protein.
- 6.4 Applications of supramolecular complexes in medicine- targeted drug delivery.

**References**

1. M.B. Smith, *Organic Synthesis*, 3<sup>rd</sup> Edn., Wave function Inc., 2010.
2. F.A. Carey, R. I. Sundberg, *Advanced Organic Chemistry*, Part A and B, 5<sup>th</sup> Edn., Springer, 2007.



3. S. Warren, P. Wyatt, *Organic Synthesis: The Disconnection Approach*, 2<sup>nd</sup> Edn., Wiley, 2008.
4. [www.arkat-usa.org](http://www.arkat-usa.org) (Retrosynthesis of D-luciferin).
5. I. Ojima, *Catalytic Asymmetric Synthesis*, 3<sup>rd</sup> Edn., John Wiley & Sons, 2010.
6. W. Carruthers, I. Coldham, *Modern Methods of Organic Synthesis*, 4<sup>th</sup> Edn., Cambridge University Press, 2004.
7. J. Clayden, N. Greeves, S. Warren, P. Wothers, *Organic Chemistry*, Oxford University Press, 2001.
8. R. Noyori, *Asymmetric Catalysis in Organic Synthesis*, John Wiley & Sons, 1994.
9. L. Kuerti, B. Czako, *Strategic Applications of Named Reactions in Organic Synthesis*, Elsevier Academic Press, 2005.
10. R.O.C. Norman, J. M. Coxon, *Principles of Organic Synthesis*, 3<sup>rd</sup> Edn., Chapman and Hall, 1993.
11. V. K. Ahluwalia, L. S. Kumar, S. Kumar, *Chemistry of Natural Products*, CRS Press, 2007.
12. J.M. Lehn, *Supramolecular Chemistry: Concepts and Perspectives*, VCH, 1995.

### SEMESTER III

#### 20P3CHET11 : PHYSICAL CHEMISTRY - III

**Credit: 4**

**Contact Lecture Hours: 72**

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

	<i>Course Outcome</i>	<i>POs / PSOs</i>	<i>CL</i>	<i>KC</i>	<i>Class Sessions</i>
<b>CO1</b>	Apply the principles of chemical kinetics in different types of reactions.	PO 1 PSO 3	U	C	27
<b>CO2</b>	Describe the chemistry of surfaces and its applications in colloids and macromolecules.	PO 1 PSO 1	U	F	27

CO3	Explain the chemistry of crystalline solids	PO 1 PSO 1	U	F	18
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**Unit 1: Chemical Kinetics****(27 Hrs)**

- 1.1 *Theories of reaction rates*: Collision theory, kinetic theory of collisions, steric factor potential energy surfaces. Conventional transition state theory, thermodynamic formulation of the reaction rate-Eyring equation. Comparison of the two theories. Significance of  $\Delta G^\ddagger$ ,  $\Delta H^\ddagger$  and  $\Delta S^\ddagger$ , volume of activation. Effect of pressure and volume on velocity of gas reactions.
- 1.2 *Unimolecular reactions*: Lindemann - Hinshelwood mechanism, qualitative idea of RRKM theory.
- 1.3 *Chain reactions*: Chain initiation processes, steady state treatment, kinetics of  $H_2-Cl_2$  and  $H_2-Br_2$  reactions, Rice-Herzfeld mechanism for decomposition of ethane and acetaldehyde, Goldfinger-Letort-Niclausse rules, branching chains, Semenov- Hinshelwood mechanism of branching chains, upper and lower explosion limits, the  $H_2-O_2$  reaction, kinetics of step growth, free radical, cationic and anionic polymerization reactions.
- 1.1 *Fast reactions*: Relaxation, flow and shock methods, flash photolysis, NMR and ESR methods of studying fast reactions.
- 1.5 *Reactions in solution*: Factors determining reaction rates in solutions, effect of dielectric constant and ionic strength, cage effect, Bronsted-Bjerrum equation, primary and secondary kinetic salt effect.
- 1.6 *Acid-base catalysis*: Specific and general catalysis, Skrabal diagram, Bronsted catalysis law, prototropic and protolytic mechanism with examples, acidity function.
- 1.7 Enzyme catalysis and its mechanism, Michelis-Menten equation, effect of pH and temperature on enzyme catalysis.
- 1.8 Introduction to oscillating chemical reactions: autocatalysis, autocatalytic mechanism of oscillating reactions, the Lotka-Volterra mechanism, the brusselator, the oregonator, bistability.

**Unit 2: Surface Chemistry****(27 Hrs)**

- 2.1 Different types of surfaces, thermodynamics of surfaces, Gibbs adsorption equation and its verification, surfactants and micelles, surface films, surface pressure and surface potential and their measurements and interpretation.
- 2.2 Application of low energy electron diffraction and photoelectron spectroscopy, ESCA and Auger electron spectroscopy, scanning probe microscopy-AFM and STM, ion scattering, SEM and TEM in the study of surfaces.

- 2.3 Surface Enhanced Raman Scattering, surfaces for SERS studies, chemical enhancement mechanism, surface selection rules, principle and application of SERS in surface chemistry.
- 2.4 *Adsorption*: The Langmuir theory, kinetic and statistical derivation, multilayer adsorption-BET theory, Use of Langmuir and BET isotherms for surface area determination. Application of Langmuir adsorption isotherm in surface catalysed reactions, the Eley-Rideal mechanism and the Langmuir-Hinshelwood mechanism, flash desorption.
- 2.5 *Colloids*: Structure and stability, the electrical double layer, zeta potential, electrokinetic phenomena - sedimentation potential and streaming potential, Donnan membrane equilibrium.
- 2.6 *Macromolecules*: Different averages, methods of molecular mass determination - osmotic, viscosity, sedimentation and light scattering methods.

### Unit 3: Crystallography

(18 Hrs)

- 3.1 Miller indices, point groups (derivation not expected), translational symmetry, glide planes and screw axes, space groups, simple cases like triclinic and monoclinic systems, interplanar spacing and method of determining lattice types, reciprocal lattices, methods of characterizing crystal structure, rotating crystal method, powder X-ray diffraction method, determination of structure of sodium chloride by powder method, comparison of the structures of NaCl and KCl, brief outline of single crystal X-ray diffraction and crystal growth techniques.
- 3.2 *Structure factor*: Atomic scattering factor, coordinate expression for structure factor, structure by Fourier synthesis.
- 3.3 *Liquid crystals*: Mesomorphic state, types, examples and application of liquid crystals.

### References

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

**SEMESTER III****20P3CHET12 : SPECTROSCOPIC METHODS IN CHEMISTRY****Credit: 3****Contact Lecture Hours: 54**

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

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

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

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

- 1.2 Influence of substituent, ring size and strain on spectral characteristics. Solvent effect, Stereochemical effect, non-conjugated interactions. Chiro-optical properties - RD, CD, octant rule, axial haloketone rule, Cotton effect-applications.
- 1.3 Problems based on the above topics.

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

- 2.1 Fundamental vibrations, characteristic regions of the spectrum (fingerprint and functional group regions), influence of substituent, ring size, hydrogen bonding, vibrational coupling and field effect on frequency, determination of stereochemistry by IR technique.
- 2.2 IR spectra of C=C bonds (olefins and arenes) and C=O bonds.
- 2.3 Problems on spectral interpretation with examples.

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

- 3.1 Magnetic nuclei with special reference to  $^1\text{H}$  and  $^{13}\text{C}$  nuclei. Chemical shift and shielding/deshielding, factors affecting chemical shift, relaxation processes, chemical and magnetic non-equivalence, local diamagnetic shielding and magnetic anisotropy.  $^1\text{H}$  and  $^{13}\text{C}$  NMR scales.
- 3.2 Spin-spin splitting: AX, AX<sub>2</sub>, AX<sub>3</sub>, A<sub>2</sub>X<sub>3</sub>, AB, ABC, AMX type coupling, first order and non-first order spectra, Pascal's triangle, coupling constant, mechanism of coupling- Dirac model. Karplus curve, quadrupole broadening and decoupling, homotopic, enantiotopic and diastereotopic protons, virtual coupling, long range coupling. NOE and cross polarization.
- 3.3 Simplification non-first order spectra to first order spectra: shift reagents, spin decoupling and double resonance, off resonance decoupling. Chemical shifts and homonuclear/heteronuclear couplings. Basis of heteronuclear decoupling.
- 3.4 2D NMR and COSY, HOMOCOSY and HETEROCOSY
- 3.5 Polarization transfer, selective population inversion, DEPT., sensitivity enhancement and spectral editing, MRI.
- 3.6 Problems on spectral interpretation with examples

**Unit 4: Mass Spectrometry (9 Hrs)**

- 4.1 Molecular ion: Ion production methods (EI). Soft ionization methods: SIMS, FAB, CA, MALDI-TOF, PD, field desorption electrospray ionization, fragmentation patterns polyenes, alkyl halides, alcohols, phenols, aldehydes and ketones, esters), nitrogen and ring rules, McLafferty rearrangement and its applications, HRMS, MS-MS, LC-MS, GC-MS.
- 4.2 Problems on spectral interpretation with examples.

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

- 5.1 Identification of structures of unknown organic compounds based on the data from UV-Vis, IR,  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR spectroscopy (HRMS data or Molar mass or molecular formula may be given).
- 5.2 Interpretation of the given UV-Vis, IR and NMR spectra.
- 5.3 Spectral analysis of the following reactions/functional transformations:
1. Pinacol-Pinacolone rearrangement
  2. Benzoin condensation
  3. (4+2) cycloaddition
  4. Beckmann rearrangement
  5. Cis-trans isomerisation of azo compounds
  6. Benzil-benzilic acid rearrangement
  7. Fries rearrangement

#### References:

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

**SEMESTER IV  
ELECTIVE COURSES**

**20P4CHET13EL : ADVANCED INORGANIC CHEMISTRY**

**Credit: 4**

**Contact Lecture Hours: 90**

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

	<i>Course Outcome</i>	<i>POs / PSOs</i>	<i>CL</i>	<i>KC</i>	<i>Class Sessions</i>
<b>CO1</b>	Apply the principles of group theory in co-ordination complexes.	PO 1 PSO 3	A	C	27
<b>CO2</b>	Identify the structure of an inorganic solid using IR, Raman, Mossbauer and EPR spectroscopic techniques.	PO 1 PSO 3	A	C	9

<b>CO3</b>	Explain the concepts of inorganic photochemistry.	PO 1 PSO 1	U	C	9
<b>CO4</b>	Describe the structure and properties of nanomaterials.	PO 1 PSO 1	R	F	18
<b>CO5</b>	Explain the chemistry of acids, bases, non-aqueous solvents and metal-organic frameworks.	PO 1 PSO 1	R	F	18
<b>CO6</b>	Explain the chemistry of fullerenes and metallo-supramolecular structures.	PO 1 PSO 1	R	F	9

**Unit 1: Applications of Group Theory****(27 Hrs)**

- 1.1 Transformation properties of atomic orbitals, hybridization schemes for sigma and pi bonding with examples, symmetry adapted linear combination of atomic orbitals in tetrahedral, octahedral and sandwich complexes - ferrocene, formation of symmetry adapted group of ligand, MO diagrams.
- 1.2 Ligand field theory, splitting of *d* orbitals in different environments using group theoretical considerations, construction of energy level diagrams, correlation diagrams, method of descending symmetry, splitting terms for orbitals, energy levels, *d-d* transition-selection rules.
- 1.3 Determination of modes of vibrations in IR and Raman spectra using character tables in tetrahedral, octahedral and square planar complexes.

**Unit 2: Inorganic Spectroscopic Methods****(9 Hrs)**

- 2.1 *Infrared and Raman Spectroscopy*: Structural elucidation of coordination compounds containing the following molecules/ions as ligands-NH<sub>3</sub>, H<sub>2</sub>O, CO, NO, OH<sup>-</sup>, SO<sub>4</sub><sup>2-</sup>, CN<sup>-</sup>, SCN<sup>-</sup>, NO<sub>2</sub><sup>-</sup> and X<sup>-</sup> (X=halogen). Use of isotopes in interpreting and assigning vibrational spectra.
- 2.2 *Electron Paramagnetic Resonance Spectroscopy*: EPR of *d*<sup>1</sup> and *d*<sup>9</sup> transition metal ions in cubic and tetragonal ligand fields, evaluation of *g* values and metal hyperfine coupling constants, electron-electron interactions, multiple resonance.
- 2.3 *Mössbauer Spectroscopy*: Applications of Mössbauer spectroscopy in the study of Fe(III) complexes. Compound Identification- the interhalogen compound I<sub>2</sub>Br<sub>2</sub>Cl<sub>4</sub>, iron in very high oxidation states – Fe(V) and Fe(VI) nitride complexes.

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



- 3.1 Excited states in transition metal complexes: Intra-ligand excited states and metal centred excited states. Photochemical reactions: Substitution and redox reactions of Cr(III), Co(III), Rh(III) and Ru(II) complexes, manganese-based photosystems for the conversion of water into oxygen, applications-synthesis and catalysis, chemical actinometry and photochromism, metal-metal multiple bonds, dissociative photochemistry, ligand loss.
- 3.2 Metal complex sensitizers, electron relay, semiconductor supported metal oxide systems, water photolysis, nitrogen fixation and CO<sub>2</sub> reduction, dinitrogen splitting.

**Unit 4: Nanomaterials****(18 Hrs)**

- 4.1 *Inorganic nanomaterials*: General introduction to nanomaterials, synthesis and applications of nanoparticles of gold, silver, rhodium, palladium and platinum, synthesis and applications of metal oxides of transition and non-transition elements-SiO<sub>2</sub>, TiO<sub>2</sub>, ZnO, Al<sub>2</sub>O<sub>3</sub>, iron oxides and mixed metal oxide nanomaterials, non-oxide inorganic nanomaterials, porous silicon nanomaterials- fabrication and chemical and biological sensing applications.
- 4.2 *Characterisation of Nanomaterials*: UV-visible, Raman, XRD, SEM, TEM and AFM techniques.
- 4.3. *Diversity in Nanosystems*: Self-assembled monolayers on gold-growth process and phase transition, gas phase clusters- formation, detection and analysis, quantum dots preparation, characterization and applications, nanoshells-types of systems, characterization and application, inorganic nanotubes-synthetic strategies, structures, properties and applications. Nanocomposites- natural nanocomposites, polymer nanocomposites, metal and ceramic nanocomposites and clay nanocomposites.
- 4.4. *Evolving Interfaces of Nanotechnology*: Nanobiotechnology, nano-biosensors, nanotechnology for manipulation of biomolecules- optical tweezers, dielectrophoresis, biochips, labs on chips, and integrated systems, nanocatalysts, nanomedicines- importance of nanomaterials in the pharmaceutical industry and future possibilities for medical nanotechnology, nanoparticles for medical imaging, nanoparticles for targeting cancer cells, nanoencapsulation for drug delivery to tumours.

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

- 6.1 Acid base concept in non-aqueous media-HSAB concept, solvent effects, linear free energy relationship-mechanism and methods of determination
- 6.2 Reactions in non-aqueous solvents. Ammonia - solutions of metals in liquid ammonia. Protic solvents: anhydrous sulfuric acid, hydrogen halides. Aprotic solvents: non-polar solvents, non-ionizable polar solvents, polar solvents undergoing autoionization, liquid halogens, interhalogen compounds, oxy halides, dinitrogen tetroxide, sulphur dioxide

**Unit 6: Metal Organic Frame Works****(9 Hrs)**

- 6.1 Introduction, porous coordination polymers, frameworks with high surface area, Lewis acid frameworks, soft porous crystals, design of metal organic frameworks and design of functional metal organic frameworks by post-synthetic modification.
- 6.2 Applications of metal organic frameworks- separation and purification of gases by MOFs, hydrogen storage, MOFs in the pharmaceutical world.

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

- 5.1 Coordination Chemistry of Fullerenes. Fullerene metal complexes-Fullerides of alkali metals, Fullerenes as  $\pi$ -ligands, Metal fullerides, exohedral fullerenes, endohedral fullerenes. (*Only elementary study is expected*)
- 5.2 Metallo supra molecular chemistry and Molecular Architecture. Molecular recognition. Molecular Receptors and selective complexation for cation, anion and neutral molecules, Supramolecular Assistance in the Synthesis of Molecular and Supramolecular structures.
- 5.3 Diamondoid networks, inorganic crystal engineering using hydrogen bonds, organometallic crystal engineering, supramolecular self-assembly caused by ionic interactions- hydrocarbyls, amides and phosphides.

**References**

1. F. A. Cotton, *Chemical Applications of Group Theory*, Wiley-Interscience, 1990.
2. V. Ramakrishnan, M. S. Gopinathan, *Group Theory in Chemistry*, Vishal Pub., 1985.
3. A. S. Kunju, G. Krishnan, *Group Theory and its Applications in Chemistry*, PHI Learning, 2010
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8. R. C. Evans, P. Douglas, H. D. Burrows, *Applied Photochemistry*, Springer, 2013.
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16. David Farrusseng, *Metal-Organic Frameworks*. Wiley-VCH, 2011.
17. Fahmina Zafar and Eram Sharmin, *Metal-Organic Frameworks*, ExLi4EvA, 2016.

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20. J. E. Mark, H. R. Alcock, R. West, *Inorganic Polymers*, 2<sup>nd</sup> Edition, Oxford University Press, 2005.

**SEMESTER IV  
ELECTIVE COURSES**

**20P4CHET14EL : ADVANCED ORGANIC CHEMISTRY**

**Credit: 4**

**Contact Lecture Hours: 90**

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

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

### Unit 1: Biosynthesis and Biomimetic Synthesis

(15 Hrs)

- 1.1 Basic principles of the biosynthesis of terpenes, steroids, alkaloids, carbohydrates, and nucleic acids.
- 1.2 Biosynthesis of cholesterol, morphine, glucose and phenyl alanine.
- 1.3 Biogenesis of isoprenoids and alkaloids. Biomimetic synthesis of progesterone and spatreine.
- 1.4 Structure of DNA and RNA. Replication of DNA - Flow of genetic information - Protein biosynthesis - transcription and translation - Genetic code - regulation of gene expression

### Unit 2: Green Alternatives to Organic Synthesis

(12 Hrs)

- 2.1 Principles of Green Chemistry: Basic concepts, atom economy - twelve principles of Green Chemistry - principles of green organic synthesis.
- 2.2 Green alternatives to Organic Synthesis: Coenzyme catalysed reactions -thiamine catalyzed benzoin condensation. Green alternatives of molecular rearrangements: Pinacol-pinacolone and Benzidine rearrangement. Electrophilic aromatic substitution reactions. Oxidation-reduction reactions. Clay catalysed synthesis. Condensation reactions. Green photochemical reactions.
- 2.3 Green Solvents: Ionic liquids, supercritical CO<sub>2</sub>, fluoros chemistry.
- 2.4 General principles of microwave and ultrasound assisted organic synthesis.

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

- 3.1 Degree of polymerization, classification and stereochemistry of polymers. Ziegler-Natta catalyst. Glass transition temperature of polymers, factors affecting glass transition temperature. Natural and synthetic rubber (SBR, Butyl, neoprene and nitrile rubber), vulcanization.
- 3.2 *Conducting polymers* - temperature resistant and flame retardant polymers - polymers for medical applications.
- 3.3 *Dendrimers and dendritic polymers*: Terminology- classification of dendrimers. Methods of synthesis: convergent and divergent approaches. Dendrimers as nanocapsules. Applications of dendrimers.
- 3.4 *Hyper branched polymers*: definition, synthesis, applications.

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

- 4.1 *Assymmetric induction*- chiral auxiliaries and chiral pool.
- 4.2 *Enantioselective catalytic hydrogenation* developed by Noyori and Knowles.
- 4.3 *Assymmetric aldol condensation* pioneered by Evans.
- 4.4 *Assymmetric Diels- Alder reactions*.
- 4.5 *Assymmetric epoxidation* using Jacobsen's catalyst.

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

- 5.1 Synthesis of camphor, atropine, papaverine, cyanin, quecertin,  $\beta$ -carotene, testosterone, PGE<sub>2</sub> and PGF<sub>2 $\alpha$</sub> , Vitamine C and Riboflavin.
- 5.2 Methods for primary structure determination of peptides, proteins.
- 5.3 Enzymes- classification, structure and mode of action.

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

- 6.1 Drug - Structure-activity relationships - a general idea.
- 6.2 *Drug action - drug selectivity- receptor proteins- drug-receptor interaction - drug metabolism. Drug-receptor theory: occupancy theory, rate theory, induced fit theory, activation-aggregation theory. Mechanism of drug acting on DNA- intercalating agent (proflavin), alkylating agent (uracil mustard, cis-platin), chain cutting agents (bleomycin).*
- 6.3 Central nervous system acting drugs (general idea), antidepressants, tranquilizers, sedatives and hypnotics.
- 6.4 A general idea of cardio-vascular drugs.
- 6.5 *Introduction to Drug design- Concept of combinatorial and parallel synthesis. Computer assisted drug design. Illustration of drug development through a specific example of antibacterials- Pencillines.*

**Unit 7: Research Methodology of Chemistry (10 Hrs)**

- 7.1 The search of knowledge - purpose of research - scientific methods - role of theory -
- 7.2 Characteristics of research. Types of research: Fundamental research, applied research, historical and experimental research.
- 7.3 *Statistical Calculations*: Presentation of data, mean, median, mode, errors in chemical analyses, linear regression and correlation. Method of least squares.
- 7.4 *Chemical Literature*: Primary, secondary and tertiary sources of literature. Classical and comprehensive reference. Literature databases: Science Direct, SciFinder. Chemical Abstract.
- 7.5 *Scientific Writing*: Research reports, thesis, journal articles, books. Types of publications: articles, communications, reviews.
- 7.6 Important scientific journals- important Chemistry journals. Impact factor

## References

1. J. M. Lehn, *Supramolecular Chemistry: Concepts and Perspectives*, VCH, 1995.
2. F. Vogtle, *Supramolecular Chemistry: An Introduction*, Wiley, 1993.
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5. R. O. C. Norman, J. M. Coxon, *Principles of Organic Synthesis*, Blackie Academic and Professional, 1993.
6. V. K. Ahluwalia, *Green Chemistry*, Ane Books, 2009.
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8. A. L. Lehninger, D.L. Nelson, M.M. Cox, *Lehninger Principles of Biochemistry*, 5<sup>th</sup> Edn., W.H. Freeman, 2008.
9. V. K. Ahluwalia, M. Chopra, *Medicinal Chemistry*, Ane Books, 2008.
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11. T. Pradeep, *Nano: the Essentials*, Tata McGraw Hill, 2007.
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16. V. K. Ahluwalia, *Green Chemistry*, Narosa Publishing House, 2013
17. Jonathan W Steed & Jerry L Atwood, *Supramolecular Chemistry*, Wiley, 2<sup>nd</sup> Edition
18. Katsuhiko Ariga, Toyoki Kunitake, *Supramolecular Chemistry – Fundamentals and Applications*, Springer.

## SEMESTER IV

**ELECTIVE COURSES****20P4CHET15EL : ADVANCED PHYSICAL CHEMISTRY****Credit: 4****Contact Lecture Hours: 90**

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

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

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

- 1.1 Quantum yield, chemical actinometry, excimers and exciplexes, photosensitization, chemiluminescence, bioluminescence, thermoluminescence, pulse radiolysis, hydrated electrons, photostationary state, dimerization of anthracene, ozone layer in the atmosphere.
- 1.2 Principle of utilization of solar energy: solar cells, types of solar cells-amorphous silicon solar cell, cadmium telluride solar cell, copper indium gallium selenide solar cell.
- 1.3 Quenching of fluorescence and its kinetics, Stern-Volmer equation, concentration quenching, fluorescence and structure, delayed fluorescence, E-type and P-type, effect of temperature on emissions, photochemistry of environment, green house effect, two photon absorption spectroscopy, lasers in photochemical kinetics.

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

- 2.1 Instrumentation: light source, monochromator, optical filters, photomultiplier tube, polarizers, fluorescence sensing, mechanism of sensing, sensing techniques based on collisional quenching, energy transfer and electron transfer, examples of pH sensors. Novel fluorophores: long life time metal-ligand complexes.

**Unit 3: Diffraction Methods and Atomic Spectroscopic Techniques (9 Hrs)**

- 3.1 Electron diffraction of gases, Wierl's equation, Neutron diffraction method, Comparison of X-ray, electron and neutron diffraction methods.
- 3.2 Atomic absorption spectroscopy (AAS), principle of AAS, absorption of radiant energy by atoms, classification of atomic spectroscopic methods, measurement of atomic absorption, instrumentation.
- 3.3 Atomic emission spectroscopy (AES), advantages and disadvantages of AES, origin of spectra, principle and instrumentation.
- 3.4 Flame emission spectroscopy (FES), flames and flame temperature, spectra of metals in flame, instrumentation.

**Unit 4: Electrochemistry and Electromotive Force (27 Hrs)**

- 4.1 Theories of ions in solution, Drude and Nernst's electrostriction model and Born's model, Debye-Huckel theory, derivation of Debye-Huckel-Onsager equation, validity of DHO equation for aqueous and non-aqueous solutions, Debye-Falkenhagen effect, conductance with high potential gradients, activity and activity coefficients in electrolytic solutions, ionic strength, Debye-Huckel limiting law and its various forms, qualitative and quantitative tests of Debye-Huckel limiting equation, deviations from the DHLL, ion association, triple ions and conductance minima.
- 4.2 Electrochemical cells, concentration cells and activity coefficient determination, liquid junction potential, evaluation of thermodynamic properties, the electrode double layer, electrode-electrolyte interface, different models of double layer, theory of multilayer capacity, electro capillary, Lippmann equation, membrane potential.
- 4.3 Fuel cells- Theory and working of fuel cells- methanol fuel cell, H<sub>2</sub>-O<sub>2</sub> fuel cell and solid oxide fuel cells.
- 4.4 Corrosion and methods of prevention, Pourbaix diagram and Evans diagrams.
- 4.5 Overvoltage: hydrogen and oxygen overvoltage, theories of overvoltage, Tafel equation and its significance, Butler-Volmer equation for simple electron transfer reactions, transfer coefficient, exchange current density, rate constants.

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

- 5.1 *Voltametry*: Cyclic voltametry, ion selective electrodes, anodic stripping voltametry.
- 5.2 *Polarography*: Decomposition potential, residual current, migration current, supporting electrolyte, diffusion current, polarogram, half wave potential, limiting current density, polarograph, explanation of polarographic waves.
- 5.3 The dropping mercury electrode, advantages and limitations of DME, quantitative analysis - pilot ion procedure, standard addition methods, qualitative analysis determination of half wave potential of an ion, advantages of polarography.



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

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

## Unit 6: Advanced Thermodynamics

(9 hrs)

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

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

### References

1. K. K. Rohatgi-Mukherjee, *Fundamentals of Photochemistry*, 2<sup>nd</sup> Edn., New Age International, 1986.
2. G. Aruldas, *Molecular structure and Spectroscopy*, PHI Learning, 2007.
3. B. Valeur, *Molecular Fluorescence: Principles and Applications*, Wiley-VCH 2002.
4. J. R. Lakowicz, *Principles of Fluorescence Spectroscopy*, 3<sup>rd</sup> Edn., Springer, 2006.
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**SEMESTERS III & IV****20P4CHEP04 : INORGANIC CHEMISTRY PRACTICAL - II****Credit: 3****Contact Lab Hours: 54 + 54 =108**

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

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

**PART I**

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

**PART II**

Introduction to material science and Nanotechnology

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

**References**

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06. T. Pradeep, *Nano: the Essentials*, Tata Mc Graw Hill, 2007.
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**SEMESTERS III & IV****20P4CHEP05 : ORGANIC CHEMISTRY PRACTICAL - II****Credit: 3****Contact Lab Hours: 54 + 54 =108**

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

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

**PART I**

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

**PART II**

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

**PART III**

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

#### PART IV

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

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

#### PART V

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

#### REFERENCES

- 1 A.I.Vogel, *A Textbook of Practical Organic Chemistry*, Longman, 1989.
- 2 A.I.Vogel, *Elementary Practical Organic Chemistry*, Longman, 1957.
- 3 F.G. Mann, B.C Saunders, *Practical Organic Chemistry*, 2009.
- 4 J.R. Johnson, J.F.Wilcox, *Laboratory Experiments in Organic Chemistry*, Macmillan, 1979.
- 5 V.K. Ahluwalia, *Green Chemistry : Environmentally Benign Reactions*, Ane Books, New Delhi, 2009.
- 6 Monograph on Green Chemistry Laboratory Experiments, Green Chemistry Task Force Committee, DST, 2009.
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### SEMESTERS III & IV

#### 20P4CHEP06 : PHYSICAL CHEMISTRY PRACTICAL - II

**Credit: 3**

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

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

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

#### I Chemical Kinetics

##### 1. Determination of the rate constant of the hydrolysis of ester by sodium hydroxide/HCl

2. Determination of Arrhenius parameters.
3. Kinetics of reaction between  $K_2S_2O_8$  and KI
4. Influence of ionic strength on the rate constant of the reaction between  $K_2S_2O_8$  and KI
5. Iodination of acetone in acid medium.

## II Polarimetry

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

## III Refractometry

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

## IV Viscosity

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

## V Conductivity measurements

1. Verification of Onsager equation.
2. Determination of the degree of ionization of weak electrolytes.
3. Determination of pKa values of organic acids.
4. Determination of solubility of sparingly soluble salts.
5. Titration of a strong acid/Weak acid against a strong base.
6. Titration of a dibasic acid against a strong base.
7. Conductometric determination of the rate constant for the alkaline hydrolysis of methyl acetate.

## VI Potentiometry

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

## References

01. J.B. Yadav, *Advanced Practical Physical Chemistry*, Goel Publishing House, 2001.
02. G.W. Garland, J.W. Nibler, D.P. Shoemaker, *Experiments in Physical Chemistry*, 8<sup>th</sup> Edn. McGraw Hill, 2009.
03. B. Viswanathan, *Practical Physical chemistry*, Viva Pub., 2005
04. Saroj Kumar and Naba Kumar, *Physical Chemistry Practical*, New Central Book Agency, 2012
05. Practical Physical Chemistry Paperback, 1974 by A.M. James, F.E. Prichard.

## 16P4CHECV - Comprehensive Viva Voce

There will be a comprehensive viva at the end of the programme. The viva board consists of three external examiners preferably same as the practical examiners for the respective subject and one internal examiner (Class teacher).

## 16P4CHEPJ - Project

Each student should submit a project report for evaluation. A minimum of 3 months period shall be given to each student for the project and this may be after the end semester examination of semester

4. Students can do their project in the department or any other reputed research institution in and outside the state. After completing the project the report should be submitted to the department for internal and external evaluation. The external evaluation will be done by the project viva board, which consists of three examiners preferably same as the practical examiners for the respective subjects.