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

CURRICULUM AND SYLLABUS

of

M.Sc. APPLIED CHEMISTRY - PHARMACEUTICAL

(PG CREDIT SEMESTER SYSTEM)

INTRODUCED FROM 2021-22 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. Pharmaceutical Chemistry for the approval of Faculty, Board of Studies and Academic Council of Sacred Heart College (Autonomous) Thevara.

Chemistry is a fundamental science and has contributed immensely for the improvement of human life by providing materials, methods and other essentialities. Also, chemistry is essential to solve many future problems, including sustainable energy and food production, managing our environment, providing safe drinking water and promoting human and environmental health. The progress achieved in the fields of chemistry in the past few decades was phenomenal. It is also seen that these developments are crossing the traditional vertical boundaries of scientific disciplines. Now a chemist cannot isolate himself from other disciplines. New branches of chemistry such as computational chemistry, bioorganic chemistry, material chemistry, green chemistry etc. are emerging and gaining importance. The practise of chemistry in industry is also undergoing radical changes. It is with these visions we have revised the syllabi of the two PG courses. Also, we have followed the PG Guidelines prepared by Mahatma Gandhi University, Kottayam in this attempt. The revised syllabi will be implemented with effect from academic year 2021-22 and onwards under Choice Based Credit System (CBCS).

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

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

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

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

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

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INTRODUCTION

1.1 M.Sc. Applied Chemistry (Pharmaceutical) Programme

Applied Chemistry is the scientific field of understanding basic chemical properties of materials to synthesize new materials with suitable applications. Applied Chemistry not only provides technologies for applications but also covers fundamental aspects

The M.Sc. Applied Chemistry (Pharmaceutical) programme is a two year – four semester programme. The programme covers principles and applications of Inorganic, Organic and Physical disciplines of chemistry and the applied topics in the pharmaceutical chemistry area. Pharmaceutical Chemistry is a branch of chemistry which deals with the study of drug molecules, its structural aspects, chemical biology and pharmacology. Study of the design and synthesis of pharmaceuticals and biologically active molecules are important part of this branch. Student will gain knowledge of the subject and experience for industrial research and education through lectures, laboratory sessions, assignments, seminars and project works. The Master's degree program in Applied Chemistry (Pharmaceutical) lays the foundation for doctoral programs in Chemistry.

1.2 Eligibility Criteria for Admissions:

- The admission to all PG programmes shall be as per the rules and regulations of the college.
- The eligibility criteria for admission shall be as announced by the college from time to time.
- 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.
- There shall be provision for credit transfer subject to the conditions specified by the Board of Studies concerned.

1.3 Admission requirements:

- 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.
- The candidate must forward the enrolment form to the Controller of Examinations of the college through the Head of the Department.
- 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.
- Students admitted under this programme are governed by the Regulations in force.

II

REGULATIONS FOR POST GRADUATE PROGRAMMES UNDER CREDIT SEMESTER SYSTEM (CSS) – 2021

2.1 TITLE

These regulations shall be called '**SACRED HEART COLLEGE REGULATIONS FOR POST GRADUATE PROGRAMMES UNDER CREDIT SEMESTER SYSTEM (CSS) – 2021'**

2.2 SCOPE

Applicable to all Post Graduate (PG) programmes of the college with effect from 2021-22 admissions. The provisions herein supersede all the existing regulations for the Post Graduate programmes of the college.

2.3 DEFINITIONS

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

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

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

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

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

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

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

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

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

2.3.10 '***Programme Project*'** means a regular project work with stated credits on which the student

undergoes a project under the supervision of a teacher in the parent department / any appropriate Institute in order to submit a dissertation on the project work as specified.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

2.3.27 *'Cumulative Grade Point Average'* (CGPA) is the value obtained by dividing the sum of credit

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

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

2.4 ATTENDANCE

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

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

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

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

2.4.4 **Duty Leave**: A student representing the college in sports, arts, social service or academic matters, has to get sanction from the class teacher concerned and submit the leave application form duly endorsed by the class teacher and the Head of the Department, and submit it to the Vice Principal. The same will be forwarded by the Vice Principal for attendance entry. The approval of the Department of Physical Education and the class teacher is required for granting attendance related to sports. The time limit for submission mentioned above is applicable in the case of duty leave as well.

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

2.4.6 **Re-admission**: A student whose attendance is inadequate will have to discontinue the studies. Such students, whose conduct is good, may be re-admitted with the approval of Governing Body, on the basis of recommendation from the department, and assurance from the student

and the guardian regarding good conduct and compliance in academic and discipline matters. For this the prescribed re-admission fee has to be paid.

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

2.5 PROGRAMME REGISTRATION

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

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

2.6 PROMOTION

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

2.7 EXAMINATIONS

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

2.8 EVALUATION AND GRADING

2.8.1 Evaluation:

The evaluation scheme for each course shall contain two parts;

(a) Continuous Internal Assessment (CIA) and

(b) End Semester Examination (ESE).

25% weightage shall be given to internal evaluation and the remaining 75% to external evaluation and the ratio and weightage between internal and external is **1:3**, for the courses with or without practicals (except the courses offered by the School of Communications). In the case of courses offered by the School of Communications, the internal-external assessment ratio shall be **1:1**. In their case, the components for evaluation and their respective weightage

shall be determined by their Board of Studies. Both internal and external evaluation shall be carried out in the grading system and the GPAs are to be rounded to two places of decimals.

2.8.2 Direct Grading:

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

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

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

2.8.4 Continuous Internal Assessment (CIA)/ Continuous Assessment:

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

a) Components of Internal Evaluation (for theory)

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

b) Components of Internal Evaluation (for Practical)

Sl. No.	Components	Weightage
i.	Written / Lab Test	3
ii.	Record	1
iii.	Lab Involvement	1
iv	Viva	1
	Total	**5**

c) Components of Internal Evaluation (for Project)

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

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

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

2.8.5 Components of End Semester Examination (ESE):

a) For Theory

Evaluation shall be based on the following pattern of questions:

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

b) Components of External Evaluation (for Practical)

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

c) Components of External Evaluation (for Project)

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

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

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

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

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

ii. Project work shall be carried out under the supervision of a teacher in the concerned department or an external supervisor.

iii. A candidate may, however, in certain cases be permitted to work on the project in an industrial / Research Organization/ Institute on the recommendation of the Supervisor.

iv. There should be an internal assessment and external assessment for the project work in the ratio 1:3

v. The external evaluation of the project work consists of valuation of the dissertation (project report) followed by presentation of the work and viva voce.

2.9 PERFORMANCE GRADING

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

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

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

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

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

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

Thus, $SGPA = {}^{TCP}\!/_{TCr}$ $\quad i=1$

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

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

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

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

total credits of the programme.

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

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

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

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

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

2.10 REGISTRATION FOR THE EXAMINATION

a. All students admitted in a programme with remittance of prescribed fee are eligible for the forthcoming semester examinations.
b. Online application for registration to the various End Semester Examinations shall be forwarded to the CE along with prescribed fee for each course in prescribed format.
c. The eligible candidates who secure the prescribed minimum attendance of the total duration of the course and possess other minimum qualification prescribed in the regulations for each course shall be issued the hall tickets. The hall ticket shall be downloaded by the students from the college website.
d. The mode of fee remittance shall be through the prescribed bank.

2.11 SUPPLEMENTARY EXAMINATIONS

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

2.12 PROMOTION TO THE NEXT HIGHER SEMESTER

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

a) He / she secures a minimum 75 % attendance and registered for the End Semester Examination of the programme for which he/she is studying.
b) His / her progress of study and conduct are satisfactory during the semester completed, as per the assessments recorded by the course teachers and the Head of the Department concerned.

2.13 CERTIFICATES

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

2.14 RANK CERTIFICATE

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

2.15 AWARD OF DEGREE

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

2.16 MONITORING

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

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

2.17 GRIEVANCE REDRESSAL MECHANISM

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

Level 1: Level of the course teacher concerned

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

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

2.18 TRANSITORY PROVISION

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

PROGRAMME STRUCTURE

Course Code	Course Title	Credits	Hours / Week	Hour / Sem.	Examination		
					ESE *Duration*	**ESE** *Max. Weight*	**CIA** *Max. Weight*
SEMESTER I							
21P1CPHT01	Inorganic Chemistry - I	4	4	72	3 Hrs.	30	5
21P1CPHT02	Basic Organic Chemistry	4	4	72	3 Hrs.	30	5
21P1CPHT03	Physical Chemistry - I	3	3	54	3 Hrs.	30	5
21P1CPHT04	Quantum Chemistry & Group Theory	4	4	72	3 Hrs.	30	5
21P2CPHP01	Inorganic Chemistry Practical - I	-	3	54	*Examination at the end of Sem II*		
21P2CPHP02	Organic Chemistry Practical - I	-	3	54	*Examination at the end of Sem II*		
21P2CPHP03	Physical Chemistry Practical - I	-	4	72	*Examination at the end of Sem II*		
	Total	**15**	**25**	**450**			
SEMESTER II							
21P2CPHT05	Inorganic Chemistry - II	4	4	72	3 Hrs.	30	5
21P2CPHT06	Organic Reaction Mechanism	4	4	72	3 Hrs.	30	5
21P2CPHT07	Physical Chemistry - II	3	3	54	3 Hrs.	30	5
21P2CPHT08	Theoretical & Computational Chemistry	4	4	72	3 Hrs.	30	5
21P2CPHP01	Inorganic Chemistry Practical - I	3	3	54	6 Hrs.	15	5
21P2CPHP02	Organic Chemistry Practical - I	3	3	54	6 Hrs.	15	5
21P2CPHP03	Physical Chemistry Practical - I	3	4	72	6 Hrs.	15	5
	Total	**24**	**25**	**450**			
SEMESTER III							
21P3CPHT09	Drug Design and Pharmacology	4	4	72	3 Hrs.	30	5
21P3CPHT10	Organic Syntheses	4	4	72	3 Hrs.	30	5
21P3CPHT11	Physical Chemistry - III	4	4	72	3 Hrs.	30	5
21P3CPHT12	Spectroscopic Methods in Chemistry	3	3	54	3 Hrs.	30	5
21P4CPHP04	Pharmaceutical Analysis Practical	-	3	54	*Examination at the end of Sem IV*		
21P4CPHP05	Drug Synthesis & Dispensing Practical	-	3	54	*Examination at the end of Sem IV*		
21P4CPHP06	Biochemistry & Bacteriology Practical	-	4	72	*Examination at the end of Sem IV*		
	Total	**15**	**25**	**450**			
SEMESTER IV							
21P4CPHT13EL	Biochemistry & Bacteriology	4	5	90	3 Hrs.	30	5
21P4CPHT14EL	Advances in Pharmaceutical Operations	4	5	90	3 Hrs.	30	5
21P4CPHT15EL	Medicinal Chemistry	4	5	90	3 Hrs.	30	5
21P4CPHP04	Pharmaceutical Analysis Practical	3	3	54	6 Hrs.	15	5
21P4CPHP05	Drug Synthesis & Dispensing Practical	3	3	54	6 Hrs.	15	5
21P4CPHP06	Biochemistry & Bacteriology Practical	3	4	72	6 Hrs.	15	5
21P4CPHCV	Comprehensive Subject Viva Voce	2	-	-	30 min	15	5
21P4CPHPJ	Project Presentation & Viva	3	-	-	30 min	15	5
	Total	**26**	**25**	**450**			

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

At the end of the PG programme,

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

Programme Specific Outcomes of MSc Applied Chemistry (Pharmaceutical)

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

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

III

SYLLABUS FOR THE COURSES

SEMESTER I

21P1CPHT01: INORGANIC CHEMISTRY-I

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

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

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

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

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

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

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

Unit 2: Reactions of Organometallic Compounds (9 Hrs)

2.1 *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_N2, radical and ionic mechanisms. Reductive elimination- binuclear reductive elimination and σ-bond metathesis. Oxidative

coupling and reductive decoupling. Insertion (migration) and elimination reactions – insertions of CO and alkenes, insertion into M−H versus M−R, α, β, γ and δ 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 heterocylic compounds. The Dötz reaction.

Unit 4: Bioinorganic Compounds (18 Hrs)

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

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

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

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

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

4.4 Other Important metal containing Biomolecules.

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

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

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

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

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

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

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

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

References

1. J.E. Huheey, E.A. Keiter, R.L. Keiter, *Inorganic Chemistry Principles of Structure and Reactivity*, 4th Edn., Harper Collins College Publishers,1993.
2. F.A. Cotton, G. Wilkinson, C.A. Murillo, M. Bochmann, *Advanced Inorganic Chemistry*, 6th edition, Wiley-Interscience, 1999.
3. K.F. Purcell, J.C. Kotz, *Inorganic Chemistry*, Holt-Saunders, 1977.
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8. Sumit Bhaduri, Doble Mukesh, *Homogeneous Catalysis: Mechanism and Industrial Applications*, Wiley Interscience, 2000.
9. Astruc, D.; *Organometallic Chemistry and Catalysis*, Springer Verlag, 2007.
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11. Robert R. Crichton, *Biological Inorganic Chemistry A New Introduction to Molecular Structure and Function*, Elsevier, 2012.
12. H.J. Arnikar, *Essentials of Nuclear Chemistry*, Wiley Eastern, 1982.
13. S.N. Goshal, *Nuclear Physics*, S. Chand and Company, 2006.

SEMESTER I

21P1CPHT02 : BASIC ORGANIC CHEMISTRY

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

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

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

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

1.1 Review of basic concepts in organic chemistry: Bonding, hybridisation, MO 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 α, β- unsaturated carbonyl compounds involving electrophilic and nucleophilic addition - Michael addition, Mannich reaction, Robinson annulation.

Unit 2: Physical Organic Chemistry (9 Hrs)

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

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

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

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

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

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

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

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

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

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

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

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

5.2 Conformation and reactivity of elimination (dehalogenation, dehydrohalogenation, semipinacolic deamination and pyrolytic elimination - Saytzeff and Hofmann eliminations), substitution and oxidation of 2^{o} alcohols.

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.

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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

21P1CPHT03 : PHYSICAL CHEMISTRY - I

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

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

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

Unit 1: Classical Thermodynamics **(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 Fugacity, relation between fugacity and pressure, variation of fugacity with temperature and pressure. Activity and activity coefficient.

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

1.5 Chemical affinity and thermodynamic functions, effect of temperature and pressure on chemical equilibrium. Van't Hoff reaction isochore and isotherm.

1.6 Third law of thermodynamics, Nernst heat theorem, determination of absolute entropies using third law.

1.7 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

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2. R.P. Rastogi, R.R. Misra, *An introduction to Chemical Thermodynamics*, Vikas publishing house, 1996.
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11. M.C. Gupta, *Statistical Thermodynamics*, New age international, 2007.

SEMESTER I

21P1CPHT04 : QUANTUM CHEMISTRY AND GROUP THEORY

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

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

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

1.1 Symmetry elements and symmetry operations.

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

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

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

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

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

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

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

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

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

2.2. *Postulates of Quantum Mechanics*:

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

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

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

Expectation value postulate.

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

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

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

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

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

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

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

References

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SEMESTER II

21P2CPHT05 : INORGANIC CHEMISTRY - II

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

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

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

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

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

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

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

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

2.2 Interpretation of electronic spectra of complexes: Orgel diagrams and demerits, Tanabe Sugano diagrams, calculation of Dq, B and β (*Nephelauxetic ratio*) values, spectra of complexes with lower symmetries, charge transfer spectra, 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 multidendate ligands - formation of chelates, effect of H^+ on the rates of substitution of chelate complexes, metal ion assisted and ligand assisted dechelation.

3.3 Electron transfer reactions: Outer sphere mechanism-Marcus theory, 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 - σ-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

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SEMESTER II

21P2CPHT06 : ORGANIC REACTION MECHANISM

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

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

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

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

1.1 Review of organic reaction mechanisms with special reference to nucleophilic and electrophilic substitution at aliphatic carbon (S_N1, S_N2, SN_i, SE_1 and SE_2) elimination (E1 and E2) and addition reactions (Regioselectivity: Markovnikov's addition - carbocation mechanism, anti-Markovnikov's addition - radical mechanism). Elimination *vs* Substitution.

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

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

Unit 2: Chemistry of Carbanions (9 Hrs)

2.1 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 **(9 Hrs)**

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, β-eliminations involving cyclic transition states such as N-oxides (Cope reaction), acetates and xanthates (Chugayev reaction)

6.4 Introduction to Click reactions - Mechanism of the Huisgen Azide - Alkyne 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, 5th Edn., Springer, New York, 2007.
3. W. Carruthers and I. Coldham, *Modern Methods of Organic Synthesis*, First South Asian Edition, Cambridge University Press, 2005.
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5. http://www.organic-chemistry.org/namedreactions.
6. R.T. Morrison, R.N. Boyd, S.K. Bhatacharjee, *Organic Chemistry*,7thEdn., Pearson, New Delhi, 2011.
7. J. Clayden, N. Greeves, S.Warren, P.Wothers, *Organic Chemistry*, Oxford University Press, New York, 2004.
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9. S. Sankararaman, *Pericyclic Reactions-A Text Book*, Wiley VCH, 2005.

SEMESTER II

21P2CPHT07 : PHYSICAL CHEMISTRY - II

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

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

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

Unit 1: Foundations of Spectroscopic Techniques (3 Hrs)

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

Unit 2: Microwave Spectroscopy (6 Hrs)

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

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

Unit 3: Infrared and Raman Spectroscopy (9 Hrs)

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

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

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

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

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

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

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

5.1 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- δ 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*, 4th Edn., Tata McGraw Hill, 1994.
2. G. Aruldhas, *Molecular Structure and Spectroscopy*, Prentice Hall of India, 2001.
3. A.U. Rahman, M.I. Choudhary, *Solving Problems with NMR Specroscopy*, Academic Press, 1996.
4. D.L. Pavia, G.M. Lampman, G.S. Kriz, *Introduction to Spectroscopy*, 3rd Edn., Brooks Cole, 2000.
5. R.S. Drago, *Physical Methods in Inorganic Chemistry*, Van Nonstrand Reinhold, 1965.
6. R.S. Drago, *Physical Methods in Chemistry*, Saunders College, 1992.
7. W. Kemp, *NMR in chemistry-A Multinuclear Introduction*, McMillan, 1986.
8. H. Kaur, Spectroscopy, 6th Edn., Pragati Prakashan, 2011.
9. H. Gunther, *NMR Spectroscopy*, Wiley, 1995.
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Books, 1997.

11. D.N. Sathyanarayan, *Electronic Absorption Spectroscopy and Related Techniques*, Universities Press, 2001.
12. D.N. Sathyanarayana, *Vibrational Spectroscopy: Theory and Applications*, New Age International, 2007.
13. D.N. Sathyanarayana, *Introduction To Magnetic Resonance Spectroscopy ESR, NMR, NQR*, IK International, 2009.

SEMESTER II

21P2CPHT08 : THEORETICAL AND COMPUTATIONAL CHEMISTRY

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

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

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

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

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

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

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

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

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

2.1 Many-body problem and the need of approximation methods, independent particle model. Variation method: Variation theorem with proof, illustration of variation theorem using the trial function x(a-x) for particle in a 1D-box and using the trial function e-αr 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_2 molecule, singlet and triplet state functions (spin orbitals) of H2.

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

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

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

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

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

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

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

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

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

References

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

Softwares:

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

B) Ab initio, semiempirical and DFT:

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

C) Graphical User Interface (GUI):

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

SEMESTERS I & II

21P2CPHP01 : INORGANIC CHEMISTRY PRACTICAL-I

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

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

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

PART I

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

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

PART II

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

PART III

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

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

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

(c) Hexammine cobalt (III) chloride.

(d) Tetrammine copper (II) sulphate.

(e) Schiff base complexes of various divalent metal ions.

(f) Bis(dimethylglyoximato)nickel(II)

(g) Prussian blue

References

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

SEMESTERS I & II

21P2CPHP02 : ORGANIC CHEMISTRY PRACTICAL - I

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

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

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

PART I

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

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

PART II

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

PART III

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

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

References

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

SEMESTERS I & II

21P2CPHP03 : PHYSICAL CHEMISTRY PRACTICAL-I

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

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

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

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

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, 8th Edn. McGraw Hill, 2009.

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

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

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

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_a of simple organic molecules and compare it with experimental values
16. Docking studies involving protein ligand interactions.
17. Calculation of electrophilicity index in hard-soft acids and bases.

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, 2nd Edn, Longman, 2001.
5. J. M. Haile (2001) *Molecular Dynamics Simulation: Elementary Methods*.

SEMESTER III

21P3CPHT09 : DRUG DESIGN AND PHARMACOLOGY

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

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

	Course Outcome	***POs / PSOs***	***CL***	***KC***	***Class Sessions***
CO1	Explain the fundamental principles of pharmacology.	PO 1 PSO 1	U	C	12
CO2	Describe the concepts of toxicology and biotransformations.	PO 1 PSO 4	U	C	12
CO3	Illustrate the structure, mechanism of action and SAR studies of anti-infective agents, chemotherapeutic agents, drugs acting on CVS, Analgesics, Antipyretic & Anti-inflammatory drugs**.**	PO 1 PSO 1	U	F	36
CO4	Describe the synthetic studies of different classes of drugs.	PO 1 PSO 1	U	C	12

Unit 1: Pharmacology (12 Hrs)

1.1 *Drugs and Drug Targets - Enzymes*: active sites, mechanism of catalysis, Enzyme inhibitors, Enzyme selectivity, Receptors ligand gated ionic channels, G-Protein coupled receptors, Kinase linked receptors. Carrier Proteins, Structural Proteins, Nucleic acids, Lipids and carbohydrates and DNA as drug targets.

1.2 *Structure Activity Relationship* - Binding interactions, Functional groups as binding groups, Concept and definition of pharmacophore.

1.3 *Pharmacokinetic Principles*: absorption, distribution, metabolism and excretion of drugs. Dose of drugs and routes of administration. Drug dosing, drug half-life, Steady state concentration, Drug tolerance, Bioavailability, Drug delivery.

1.4 *Pharmacodynamic Principles* : Examples of agonists, allosteric modulators, Antagonists, Partial agonists, Inverse agonists, Desensitization and sensitization, Tolerance and dependence, affinity, efficacy and potency.

1.5 Dose response relationships, unusual and adverse responses of drugs, structurally specific and nonspecific drugs. Ferguson's principle.

Unit 2: Toxicology and Biotransformations (12 Hrs)

2.1 Receptor theories and receptor models - rate, occupancy, induced fit, activation-aggregation and molecular perturbation theories.

2.2 General concepts of toxicity, acute, sub-acute & chronic toxicity tests, teratogenicity & carcinogenicity, LD50, ED50, MIC- anti infectives, habituation & addiction.

2.3 Biotransformations of Drugs, factors affecting biotransformation, site of biotransformations, Effect of biotransformation on the biological activity of drugs, alterations in Phase I biotransformations. Biotransformation - Oxidation, reduction, hydroxylation, hydrolysis -

illustrate reactions and mechanism with specific drugs molecules. Phase II biotransformations - gluconideration, sulfation, conjugation with glutathione, acetylation, methylation - illustrate with suitable drug molecules. Chemical and pharmacological roles of Phase I & phase II transformations.

Unit 3: Anti-infective Agents: (12 Hrs)

3.1. ***Sulphonamides***: Structure, chemistry, SAR and mechanism of action Sulfadiazine, Sulfamethoxole, Sulfones, Cotrimoxazole (*sufamethoxole + trimethoprim*), Sulfonamides.
Synthesis: Sulfadiazine, sulfamethoxole, pyrimethamine, Dapsone.

3.2. ***Antifungal agents***: Study of the drugs - Amphotericin B, Griseofulvin, Nystatin, Ketoconazole, Clotrimazole, fluconazole, 5-Flucytosine.
Synthesis: Griseofulvin, 5-Flucytosine.

3.3. ***Antiprotozoal agents***: Chemistry, mechanism of action and therapeutic uses of Anti Amoebic and Antihelmintics.

3.4 ***Antiviral agents***: Antiviral drugs - mode of action and therapeutic uses, Chemistry and mechanism of action of : Amantadine, Ribavirin, Abacavir, Adefovir, Acyclovir, Oseltamivir, Vidarabine, Ganciclovir, Didanosine, Combivir.
Synthesis: Acyclovir, Adefovir, Ganciclovir, Didanosine, Combivir

Unit 4: Drugs acting on CVS (12 Hrs)

Pharmacology and SAR, recent advances of the following classes of drugs

4.1 ***Cardiotonic Drugs***: Cardiac Glycosides - Digoxin, Digitoxin, Dobutamine and Milrinone.
Synthesis: Milrinone

4.2 ***Antiarrhythmic Drugs***: Quinidine, Procainamide, Disopyramide, Lidocaine, Phenytoin, Propranolol, Verapamil, Bretylium.
Synthesis: Lidocaine, Phenytoin and Bretylium.

4.3 ***Antihypertensive Drugs***: Peripheral antiadrenergics - Prazosin and Terazosin, Centrally acting agents - Clonidine and Methyldopa, β-adrenergic blockers - Atenolol and Labetalol. Calcium channel blockers - Nifedipine and Amlodipine. ACE inhibitors - Captopril. Angiotensin receptor blockers - Losartan. Miscellaneous - Thiazide diuretics.
Synthesis: Captopril, Methyldopa, Amlodipine.

4.4 ***Antianginal Drugs***: Vasodilators - nitrites and nitrates, β-blockers - propranolol. Calcium channel blockers - verapamil and nifedipine. Miscellaneous - Dipyridamol and Aspirin.
Synthesis: Verapamil

4.5 ***Anticoagulants***: Heparin, Coumarin derivatives and Indanedione derivatives.

4.6 ***Antihyperlipidemic Agents***: Statins - lovastatin, simvastatin, fluvastatin. Fibrates - clofibrate, and cholestyramine resin, Dicoumarol.
Synthesis: Fluvastatin

Unit 5: Chemotherapeutic Agents (12 Hrs)

5.1 ***Antibiotics***: Classification, mechanism of action and therapeutic uses - Penicillin, Cephalosporins, Quinolones, Aminoglycosides, Carbapenems, Macrolide and others. Antibiotic resistance mechanism and implications in therapeutics.
Synthesis: Penicillin V, Cefotaxim, Meropenem, Streptomycin, Ciprofloxacin, Trimethoprim.

5.2. ***Chemotherapy of Tuberculosis***: First line drugs and second line drugs – Chemistry and pharmacology. The problem of MDR tuberculosis.
Synthesis: Isoniazid, Pyrazinamide, Ethionamide, *p*-Aminosalicylic acid.

5.3. ***Chemotherapy of Malaria***: Mode of action of the various classes of drugs used, Chemistry, SAR and Drug resistance. Study of the following drugs in the treatment, efficacy, problem of side effects – Quinine sulphate, Chloroquine, primaquine, mephloquine, quinacrine, proguanil, plaquenil. Drug combinations in the therapy of Malarial parasite. Treatment of drug resistant malaria.
Synthesis: Chloroqine, primaquine, proguanil.

Unit 6: Analgesics, Antipyretic & Anti-inflammatory drugs (12 Hrs)

***Mechanism of Action and SAR of*:**

6.1 Different types of analgesia.

6.2 ***Narcotic Analgesics***: Morphine and codeine, phenyl(ethyl)piperidines, Diphenylheptanones, fentanyl analogues, nalfurafine.
Synthesis: Codeine, Levorphanol, Pethidine and Methadone

6.3 ***Antipyretics and NSAIDs***: Basic idea of COX I & II Inhibitors, Salicylates – aspirin; *p*-aminophenol derivatives – paracetamol and phenacetin; Pyrazolidine diones – Phenylbutazone; Anthranilic acid derivatives – flufenamic acid; Indoleacetic acid derivatives – Indomethacin; Arylacetic/propionicacid derivatives - ibuprofen, ketoprofen, flubiprofen and diclofenac; Oxicams – tenoxicam
Synthesis: Phenyl butazone, flufenamic acid, diclofenac, tenoxicam, Ketoprofen

6.4 ***Drugs used for Gout*** - Allopurinol, Colchicine, Pegloticase
Synthesis: Allopurinol

6.5 ***Anti-inflammatory Agents***: Sulindac, Naproxen
Synthesis: Naproxen

6.6 ***Novel Analgesics***: Funapide, Raxatrigine (*Structure only*).

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SEMESTER III
21P3CPHT10 : ORGANIC SYNTHESES

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

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

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

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

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

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

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

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SEMESTER III
21P3CPHT11 : PHYSICAL CHEMISTRY - III

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

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

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

Unit 1: Chemical Kinetics **(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 $\Delta G^{\neq}$, $\Delta H^{\neq}$ and $\Delta S^{\neq}$, 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, Goldfingr-Letort-Niclause 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.

1.4 *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 oreganator, 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, glideplanes 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

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2. K.J. Laidler, *Chemical kinetics*, 3rd Edn., Harper & Row, 1987.
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SEMESTER III

21P3CPHT12 : SPECTROSCOPIC METHODS IN CHEMISTRY

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

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

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

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

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

1.2 Influence of substituent, ring size and strain on spectral characteristics. Solvent effect, 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}H and ^{13}C nuclei. Chemical shift and shielding/deshielding, factors affecting chemical shift, relaxation processes, chemical and magnetic non-equivalence, local diamagnetic shielding and magnetic anisotropy. ^{1}H and ^{13}C NMR scales.

3.2 Spin-spin splitting: AX, AX_2, AX_3, A_2X_3, AB, ABC, AMX type coupling, 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}H NMR and ^{13}C NMR spectroscopy (HRMS data or Molar mass or molecular formula may be given).

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

5.3 Spectral analysis of the following reactions/functional transformations:

1. Pinacol-Pinacolone rearrangement
2. Benzoin condensation
3. (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*, 3rd Edn., Brooks Cole, 2000.
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8. D. H. Williams, I. Fleming, *Spectroscopic Methods in Organic Chemistry*, 6th Edn., McGraw-Hill, 2008.
9. W. Kemp, *Organic Spectroscopy*, 2nd Edn., Macmillan, 1987.
10. F. Bernath, *Spectra of Atoms and Molecules*, 2nd Edn., Oxford University Press, 2005.
11. Online spectral databases including RIO-DB.

SEMESTER IV
ELECTIVE COURSES

21P4CPHT13EL : BIOCHEMISTRY AND BACTERIOLOGY

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

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

	Course Outcome	*POs / PSOs*	*CL*	*KC*	*Class Sessions*
CO1	Describe the structure and functions of biomolecules, amino acids, proteins, enzymes, nucleic acids and hormones.	PO 1 PSO 1	U	C	54
CO2	Explain the chemical processes involved in the biological oxidation and metabolism.	PO 1 PSO 4	U	C	18
CO3	Illustrate the application of buffer systems in pharmaceutical chemistry.	PO 1 PSO 1	A	C	6
CO4	Describe the principles of microbiology and immunology	PO 1 PSO 1	U	C	12

Unit 1: Biomolecules an over view **(6 Hrs)**

1.1 Carbohydrates, proteins, glycoprotein and Lipids and their relevance in Pharmaceutical chemistry.

1.2 Structure of cell membrane.

Unit 2: **Amino Acids and Proteins** **(12 Hrs)**

2.1 Structural and functional classification of proteins. Structure, Physicochemical properties, configuration and optional properties of amino acids, Purification of proteins and amino acids, sequence determination. Primary, Secondary Tertiary and Quaternary structure of Proteins. Protein folding, three dimensional structure of proteins. Solid phase peptide synthesis.

Unit 3: Enzymes **(18 Hrs)**

3.1 *Enzymes*: Classification, Mechanism of enzymatic reactions, kinetics of enzymatic reactions, Michaelis Menton model, Measurement of significance of Kmax and Vmax perfect enzymes. Inhibition of enzymetic reactions. Kinetics of competitive and non-competitive Inhibition. Allosteric enzymes, Mechanism of enzymatic catalysis by Lysozyme and carboxypeptidase, Zymogens.

3.2 *Coenzymes*: Classification, Structure and Function of Nicotinamide adenine dinucleotides (NAD and NADP), Riboflavin Nucleotides (FMN and FAD), Biological oxidation and reduction, Lipoic acid, Cytochromes, Pyridoxal phosphate, Nucleoside diphosphates. Tetrahydrofolic acid conjugates, Biotinyl coenzyme. Conenzyme - A, and Thiamine pyrophosphate.

3.3 *Biotechnological Application of Enzymes*: Application of immobilized enzymes, use of enzymes as targets for drug design. Clinical uses of enzyme therapy, Enzymes and recombinant DNA technology. Genomic Library.

Unit 4: Nucleic acids and Hormones (18 Hrs)

4.1 ***Nucleic acids****:* Nucleoid bases, Nucleosides, nucleotides, structure of DNA, RNA and its classifications, Replication of DNA, transcription, translation and Protein Biosynthesis. DNA finger printing Techniques, Introduction to Recombinant DNA technology. Genetic code, gene therapy (*basic concept only*), PCR. Chemical Synthesis of Nucleotides, Restriction enzymes. Chemistry of ATP, ADP and AMP.

4.2 ***Hormones****:* Functions and mode of action of hormones, Pituitary, thyroid, parathyroid, adrenal and adrenocorticoid and pancreatic hormones. Male and female sex hormones. Anti-hormones.

Unit 5: Biological Oxidation and Metabolism: (18 Hrs)

5.1 ***Carbohydrate Metabolism*:** Carbohydrate the source of energy, glycolysis, glycogenesis, pentose pathway, citric acid and Cori cycle. Regulation of carbohydrate metabolism, Hormonal regulation of carbohydrate metabolism. Fructose and Galactose metabolism. Diabetes-Type I & II.

5.2 ***Lipid Metabolism***: Oxidation of fatty acid, biosynthesis of fatty acids, Prostaglandins-classification, structure and biosynthesis and biological role.

5.3 ***Protein and Amino Acid Metabolism***: Oxidative deamination and transamination reactions, Urea formation- ornithine cycle.

Unit 6: Buffer Systems (6 Hrs)

6.1 Buffer in pharmaceutical and biological system, pH, the buffer equation (Henderson Hesselbach), Buffer calculations, three important buffer systems in human body, buffer capacity, osmotic pressure and tonicity, pharmaceutical buffers, preparations of pharmaceutical buffer solutions.

Unit 7: Microbiology and Immunology (12 Hrs)

7.1 ***Microbial Drug Development*:** Introduction to Microbiology and classification of Microbes. Characterization and Screening of Microbes: Microbia1growth, kinetics, Isolation and Improvement of Individual micro-organism, Fermentation technology: Design, operation and characteristics of fermentation processes. Staining of bacteria, theories of staining. General principles of microbial control - sterilization and disinfection.

7.2 ***Immunochemistry in pharmaceutical applications***: Overview of the immune system and its role, Adaptive and innate Immunity. Immunoglobulins - classification and structure, their biological role. Immune response and the underlying mechanisms, Regulation of immune response. Hypersensitivity, immunodeficiency, Autoimmunity, Immunization, Immunosuppresants, Immunomodulators, Immunological techniques

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16. Roitt and J. Brostff, *Immunology*, D. Male (Ed), Open University, United Kingdom. 2003.
17. L. E. Cassaida Jr., *Industrial Microbiology*, New Age International Publishers, 2007.

SEMESTER IV
ELECTIVE COURSES

21P4CPHT14EL : ADVANCES IN PHARMACEUTICAL OPERATIONS

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

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

	Course Outcome	*POs / PSOs*	*CL*	*KC*	*Class Sessions*
CO1	Describe the drug delivery systems and pharmaceutical dosage forms.	PO 1 PSO 1	U	C	28
CO2	Explain preformulation studies and stability testing of drugs.	PO 1 PSO 4	R	F	10
CO3	Illustrate the application of colloids and chromatography in pharmaceutical chemistry.	PO 1 PSO 1	A	C	24
CO4	Describe the principles of forensic pharmacy.	PO 1 PSO 1	R	F	14
CO5	Explain different methods of extraction and application of radiopharmaceuticals.	PO 1 PSO 1	R	C	14

Unit 1: Pharmaceutical Dosage forms and Drug delivery Systems (10 Hrs)

1.1 An over view of different dosage forms drug delivery systems- liposomes and nanoparticle drug delivery system, biodegradable drug delivery system, controlled release system, targeted drug delivery systems, hydrogel bases drug delivery systems,

Unit 2: Formulation and Development of solid dosage forms (18 Hrs)

2.1 New materials, excipients science - diluents, disintegrants, super disintegrants. Evaluation of functional properties of excipients, co-processed materials, methods of preparation and evaluation. Coating, coating machines, coating techniques advanced coating technologies in tablet technology for product development

Specialized tablets: Formulation and evaluation of effervescent, or dispersible and chewable tablets. Formulation and manufacture of powder dosage forms for internal use. Soft and hard gelatine capsules advances in capsule manufacture, machines, processing and control. Filling equipment and filling operations, formulations, finishing, special techniques.

2.2 **Disintegration:** Disintegration, Disintegration time, factors affecting disintegration, disintegration testing of tablets.

2.3 **Dissolution:** Theories of Dissolution, dissolution models, Factors affecting dissolution rates, dissolution of different dosage forms- solids, suspensions, suppositories, controlled drug release systems.

2.4 **Micrometrics-** Introduction, Pharmaceutical importance, particle size distribution, surface area and particle volume derived properties of powder, flow properties of power and application in pharmacy, Different methods in particle size determination.

Unit 3: Preformulation studies and Stability Testing (10 Hrs)

3.1 ***Preformulation studies***: Factors affecting dissolution, bioavailability and drug absorption – pH, pka values, Partition coefficient, particle size, solubility etc. Methods to increase solubility of poorly soluble drugs. Drug release mechanisms.

3.2 ***Stability testing***: Drugs and dosage forms: Solid state drug stability, dosage form stability, accelerated stability testing, shelf life calculations, strategies for prolonging shelf life. Effect of packaging materials on dosage form stability. Photostability testing and oxidative stability, role of containers in stability testing.

Unit 4: Colloids (10 Hrs)

4.1 Pharmaceutical application of colloids, brief introduction to properties of colloids. Coarse dispersions**:** Physical stability of suspension and emulsions, types of suspension, controlled flocculation-floculated suspension, types of emulsion, theories of emulsification, emulsifying agents mechanism of action, factors to improve physical stability of emulsions.

Unit 5: Forensic pharmacy (14 Hrs)

5.1 Getting the drug to the market- Preclinical studies of toxicology, drug metabolism pharmacology, formulation and stability tests and Clinical trials

5.2 IPR: Patents: Conditions for patentable inventions, Patentable inventions under the patent Act 1970, Types of inventions not patentable in India, Term of patent in Indian System, Essential patent documents to be submitted, Provisional specification and complete specification, Criteria for naming inventors patent

5.3 Copyright Entitlement to copyright, works protected by copyright, Rights granted by copyright, Geographical indication

5.4 BP, IP, USP, Limits Tests

Unit 6: Chromatography (14 Hrs)

6.1 Applications of chromatography as an analytical and diagnostic tool in pharmaceutical chemistry-over view of plate and rate theories, different classification of chromatography,- adsorption, partition, size exclusion (GPC), Affinity, Ion exchange. Applications of PC, TLC, GC& different detectors, GCMSS, Column chromatography, HPLC. Normal and reverse phase, chiral Columns, LCMS and its applications in pharmaceutical chemistry.

Unit 7: Modern Techniques of Extraction and Radio Pharmaceuticals (14 Hrs)

7.1 Radio Pharmaceuticals and their applications in diagnosis and treatment, Diagnostics techniques- ELISA, RIA, PET, SPET

7.2. Principles and methods of Industrial extraction, evaporation and distillation, ultracentrifugation, electrophoresis.

References:

1. *Pharmaceutical drug Dosage Forms and Drug Delivery System*: Mahanto R I and Narang, CRC Press Second Edition
2. *Remington's Science and Practice of pharmacy*, Edited by Allen, Loyd V., Jr 22nd edition, 2012
3. N. K. Jain, *A Text Book of Forensic Pharmacy*, 6th Edn., Vallabh Prakashan, 2003.
4. P. Ganguli, *Intellectual Property Rights: Unleashing the Knowledge Economy*, Tata McGraw Hill, 2001.
5. D. M. Vasudevan, S. Sreekumari, V. Kannan, *Textbook of Biochemistry for Medical Students*, 6th Edn., JP Medical, 2010.

SEMESTER IV

ELECTIVE COURSES

21P4CPHT15EL : MEDICINAL CHEMISTRY

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

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

	Course Outcome	***POs / PSOs***	***CL***	***KC***	***Class Sessions***
CO1	Explain the principles of drug design and development, QSAR, CADD and combinatorial chemistry.	PO 1 PSO 1	U	C	46
CO2	Illustrate the structure and mechanism of actions of antineoplastic drugs, drugs acting on ANS and drug acting on CNS.	PO 1 PSO 4	U	C	34
CO3	Explain the synthetic studies of different classes of drugs.	PO 1 PSO 1	A	C	10

Unit 1: Drug Design and Development **(14 Hrs)**

1.1 Development of new drugs, procedures followed in drug design.

1.2 Concept of lead compounds and lead modification & lead optimization - phytochemicals as lead compounds.

1.3 Prodrugs and soft drugs. Functions and properties of prodrugs and its effect and significance with relation to pharmacological activity.

1.4 Endogenous compounds as drugs- neurotransmitters, natural hormones.

1.5 Peptidomemetics in drug design.

1.6 SAR, factors affecting bioavailability, resonance and inductive effects, isosterism, bioisosterism.

Unit 2: QSAR **(12 Hrs)**

2.1 Introduction and perspectives and parameters involved in studies of QSAR

2.2 Types of QSAR models

2.3 Classification of parameters utilized in QSAR studies

2.4 Statistical concept of QSAR

2.5 Hansch model of QSAR

2.6 De Novo model of QSAR

2.7 Hammett and Taft model of QSAR equations

2.8 Applications of QSAR in drug design

Unit 3: Computer Aided Drug Design (CADD) (10 Hrs)

3.1 Introduction to drug discovery -Target and Lead Identification -Virtual screening- concept, Ligand based and structure based. Drug Likeness – ADME, Pharmacophore Screening

3.2 Molecular modeling- Quantum mechanics and Molecular mechanics, Docking studies, Pharmacokinetics and Pharmacodynamics. Advantages of CADD.

Unit 4: Combinatorial Chemistry (10 Hrs)

4.1 Introduction

4.2 Combinatorial approaches

4.3 Peptide and small molecule libraries

4.4 Applications, methodology

4.5 Combinatorial Organic Synthesis

4.6 Assays and Screening of Combinatorial libraries

4.7 Introduction to High Throughputs Screening (HTS)

Unit 5: Antineoplastic Drugs (12 Hrs)

5.1 Cancer chemotherapy

5.2 Role of alkylating agents, antimetabolites and folate antagonists in the treatment of cancer. Carcinolytic antibiotics and mitotic inhibitors.

5.3 Plant derived drugs - vincristine, taxol

5.4 Hormones and their antagonists.

5.5 Recent developments in cancer chemotherapy-immunological intervensions

5.6 *Synthesis* : 5-flurouracil, 6-mercaptopurine, methotrexate, tamoxifen.

Unit 6: Drugs acting on ANS (14 Hrs)

6.1 Introduction to autonomic nervous system and classification.

Mechanism of action and uses of the following classes of drugs:

6.2 ***Adrenergic agonists*** : Clonidine, oxymetazoline, salbutamol. Adrenergic blockers: α and β adrenoreceptor antagonists-ergot alkaloids - Pronethalol, propranolol, atenolol, metoprolol, pindolo.

Synthesis: Salbutamol, Metoprolol,

6.3 ***Cholinergic stimulants***: nicotinic and muscarinic receptors, acetyl choline, pilocarpine and carbachol.

Synthesis: Carbachol,

6.4 ***Cholinergic blockers***: atropine, hyoscine

Synthesis: atropine

6.5. ***Nicotinic antagonists***: Decamethonium and suxamethonium

6.6 ***Anti-cholinesterases***: Competitive inhibitors-physostigmine and neostigmine. Organo phosphorous compounds and nerve gases.

Unit 7: Drugs acting on CNS: pharmacology of the following classes of drugs (18 Hrs)

7.1 Hypnotics, sedatives and anxiolytic agents.

7.2 ***Anxiolytic agents*** : Benzodiazepines, buspirone and meprobamate.

Synthesis: Enflurane, Etomidate, Meprobamate

7.3 ***Anticonvulsants***: Convulsions, types of epilepsy, barbiturates - hydantoins, oxazolidinediones, succinimides and benzodiazepines.

Synthesis: Phenobarbital, Diazepam, Chlordiazepoxide, Ethosuximide, Denzimol, Topiramate

7.4 ***Analeptics***: Xanthines, amphetamines, nikethamide and ethamivan.
Synthesis: Nikethamide, Ethamivan

7.5 ***Centrally acting muscle relaxants***: Glyceryl ethers - mephenesin, alkane diol derivatives-meprobamate, benzodiazepines-librium, diazepam and baclofen.

7.6 ***Anti-parkinson's agents***: Dopamine agonists, dopamine releasing agents and synthetic anticholinergics.

Synthesis: Levodopa, Diphenhydramine

7.7 ***Drugs for Alzheimer's disease***: Cholinergic agonists and acetylcholine esterase inhibitors.
Synthesis: Tacrine

References:

1. *Essentials of Pharmaceutical Chemistry*, Donald Carins; Pharmaceutical Press, 3 Edn.
2. *Principles of Medicinal Chemistry*, William Foye, Lippincott 5 Edn
3. *Text Book of Medicinal and Pharmaceutical Chemistry*, Wilson &Gisvold Lippincott, 10 Edn.
4. *Medicinal Chemistry & Drug Discovery*, Alfred Burger, John Wiley 6 Edn, 2007
5. *Fundamentals of Medicinal Chemistry*, G. Thomas. Wiley Publications 2006
6. *An Introduction to Medicinal Chemistry*, Graham L Patrick, Oxford University Press 2006
7. *Organic Chemistry* Vol: II, IL FINAR
8. *Natural Products Chemistry*, NR Krishnaswami, Oxford University Press, 2008
9. *Recent Progress in Medicinal Plants* Vol.I, Singh, Govil, Tec. Publications LLC, USA,2002.
10. *Computer aided Drug design*, TJ PERUN7 CL Propst, Marcel& Dekker, 2007.

11. *Introduction to Principles of Drug Design*, Smith HJ, Willims H Edn. Wright Boston
12. *Computer Aided Drug Design*, Pope & Perruns, Academic Press, NY.
13. *Heterocyclic Chemistry in Drug Discovery*, Edn, JIE Jack Li, Wiley.
14. *Organic Chemistry of Drug Design and Drug Action*, Richard B Silverman Academic Press
15. *Computational Medicinal Chemistry for Drug Discovery*, P Bultinck, P DeVinter.
16. *Medicinal Chemistry*, Alex Gringauz, Wiley India.

SEMESTERS III & IV

21P4CPHP04 : PHARMACEUTICAL ANALYSIS PRACTICAL

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

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

	Course Outcome	*POs / PSOs*	*CL*	*KC*	*Class Sessions*
CO1	Prepare different classes of drugs.	PO 1 PSO 5	A	P	54
CO2	Analyse drugs using common analytical techniques.	PO 1 PSO 5	A	P	27
CO3	Determine pKa values of drugs	PO 1 PSO 5	A	P	27

1. **Preparation, assay including limit tests** prescribed in the IP/BP of the following drugs: sodium salicylate, calcium lactate, yellow mercuric oxide, ferrous fumarate, ferric ammonium citrate, potassium antimony citrate, boric acid, light magnesium carbonate, and sodium citrate. Expectorants and emetics (NH_4Cl, antimony potassium tartarate), Respiratory Stimulants $(NH_4)_2CO_3$, Dental products (Dicalcium Phosphate, Sodium Fluoride) Gastrointestinal agents: $MgSO_4$
2. Assay, test for identity and purity of the following synthetic drugs:
   Aspirin, Paracetamol, Ibuprofen, hexamine, Boric acid, Ferrous Fumarate, Isoniacid, Calcium lactate, Calcium gluconate.
3. Analysis of official drugs using common analytical techniques (*separation of excipients from tablets and Assay using spectrophotometer*).
4. Assay of Antibiotics.
5. Assay of Vitamins: ascorbic acid, acetomenaphthone, niacinamide, pyridoxine and thiamine.
6. Determination of pKa values of drug molecules.
7. Determination of pKa values at different pH conditions

References

1. A.O. Bentley, J.E. Driver, Bentley and Driver's Textbook of Pharmaceutical Chemistry, 7th Edn., Oxford University Press, 1960.
2. G.L. Genkins, A.M. Knevel, F.E. DiGangi, Quantitative Pharmaceutical Chemistry, 7th Edn., McGraw Hill, 1977.
3. K.A. Connors, A Textbook of Pharmaceutical Analysis, John Wiley & Sons, 2007.
4. Indian Ministry of Health and Family Welfare, Indian Pharmacopoeia 1996, Controller of Publication, 2000.
5. Vogl's Text Book of Practical Organic Chemistry- Brian Furniss, Antony Hannaford, Peter Smith, Austrin (Eds), 5th edition, ELBS Publication, Singapore, 1997.

6. Experimental Pharmaceutical Organic Chemistry, A Becnchtop Manual by K. S. Jain, P. B. Miniyar & T. S. Chitre, 2nd Edition Carrier publications.
7. Organic Chemistry, G. Marc Loudon, 4th Ed., Oxford University Press, 2004.
8. British Pharmacopoeia Commission, British Pharmacopoeia:2012 Edition, Bernan Assoc, 2011

SEMESTERS III & IV
21P4CPHP05 : DRUG SYNTHESIS & DISPENSING PRACTICAL

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

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

	Course Outcome	*POs / PSOs*	*CL*	*KC*	*Class Sessions*
CO1	Synthesize typical organic medical compounds.	PO 1 PSO 5	A	P	54
CO2	Perform extraction and TLC analysis of plant extracts.	PO 1 PSO 5	A	P	27
CO3	Isolate natural products from their sources.	PO 1 PSO 5	A	P	27

1. Synthesis of some typical organic medicinal compounds, spectral illustration of the intermediates and products formed: paracetamol, sulphanilamide, hippuran, benzocaine, clofibrate, mercurochrome, phenytoin, dapsone, sulphasalazin, antipyrine, aminacrine and phenobarbitone.

2. Preparation of some specified crude plant extracts and qualitative analysis by TLC of crude plant extracts/ products to detect the presence of phytochemicals.

3. Isolation of phytochemicals from their natural sources.
   Examples Caffeine from Tea, Nicotine from tobacco, Curcumin from turmeric, Tannins from Gallnuts, Lycopene from tomato

4. Qualitative analysis of barbiturates, lactates, tartarates and alkaloids.

5. Limit tests.

References

1. A. O. Bentley, J.E. Driver, Bentley and Driver's Textbook of Pharmaceutical Chemistry, 7th Edn., Oxford University Press, 1960.
2. K.A. Connors, A Textbook of Pharmaceutical Analysis, John Wiley & Sons, 2007.
3. J.W. Cooper, C. Gunn, Cooper and Gunn's Dispensing for Pharmaceutical Students, Pitman Medical, 1967.
4. A. Kar, Advanced Practical Medicinal Chemistry, New Age International, 2007.

SEMESTERS III & IV

21P4CPHP06 : BIOCHEMISTRY AND BACTERIOLOGY PRACTICAL

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

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

	Course Outcome	***POs / PSOs***	***CL***	***KC***	***Class Sessions***
CO1	Analyse blood and urine samples.	PO 1 PSO 5	A	P	54
CO2	Estimate the amino acids by titration methods.	PO 1 PSO 5	A	P	27
CO3	Identify amino acids and peptides by PC and TLC	PO 1 PSO 5	A	P	27
CO4	Separate serum proteins by paper electrophoresis	PO 1 PSO 5	A	P	36

A. Biochemistry

1. Blood Analysis

    a. Determination of blood group and Rh factor.

    b. Enumeration of RBC, WBC and differential leucocyte count.

    c. Determination of ESR.

    d. Estimation of urea, uric acid, cholesterol, creatinine, haemoglobin and calcium.

2. Urine Analysis

    a. Qualitative analysis of urine for the common pathological constituents - sugar, albumin, ketone bodies, bile.

    b. Estimation of albumin, ketone bodies, sugar and urea.

3. Quantitative Estimation of Amino acids by formol titration and direct titration.

4. Identification of Amino acids and peptides by PC and TLC and Colour reactions

5. Separation of serum proteins by paper electrophoresis.

B. Bacteriology

1. Preparation of some typical nutrient media for collection and isolation of bacteria.

    a. Nutrient Agar, Endo's Agar, Chapman's Agar, Tergotol-7 Agar and McConkey Agar.

2. Staining and the study of the morphology of the bacteria.

a. Simple stain

b. Gram stain (Huker method)

c. Capsule stain

d. Acid fast stain (Ziehl- Neelson)

e. Negative stain (India ink method)

3. Identification of some common pathogenic organisms.

4. Enumeration of bacteria in milk-the reductase test.

5. Evaluation of germicides-Riedel Walker test.

6. Antibiotic sensitivity tests.

21P4CPHCV - Comprehensive Viva Voce

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

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

21P4CPHPJ - Project

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

IV

MODEL QUESTION PAPERS

MSc Degree End Semester Examination

Semester I: Chemistry / Pharmaceutical Chemistry

21P1CHET01 / 21P1CPHT01 – INORGANIC CHEMISTRY - I

(2021 admission onwards)

Time: Three hours Max. Weight: 30

Section- A

(Answer any **eight** questions. Each question carries a weight of 1)

1. What is synergism?
2. Define the term "isolobal".
3. Give an example for a β-elimination reaction.
4. What are Ziegler- Natta catalysts?
5. What is Bohr effect?
6. What is *cis*-platin? What are its important applications?
7. What is radiation polymerisation?
8. How is nuclear reaction cross section related to reaction rate?
9. List the important functions of biological membranes.
10. Give an example for the use of palladium catalysts in the formation of C-N bond.

(8 x 1 = 8)

Section B

(Answer any **six** questions. Each question carries a weight of **2**)

11. Discuss the bonding in ferrocene.
12. What are oxidative addition reactions? Discuss the important mechanisms involved in oxidative additions.
13. What is Wilkinson's catalyst? What are its uses? Describe alkene hydrogenation using Wilkinson's catalyst with the help of Tolman catalytic loops.
14. Explain the structure and functions of carbonic anhydrase, carboxypeptidase A and superoxide dismutase.
15. Write a note on the synthesis of transuranic elements.
16. Outline the role of chlorophyll in photosynthesis.
17. What are insertion reactions? Discuss insertion of alkenes and alkynes in the Ar-H bond.
18. Write a note on carbonyl clusters. (**6 x 2 = 12**)

Section C

(Answer any **two** questions. Each question carries a weight of 5)

19. What are π-bonding ligands? Explain the preparation, properties, structure and bonding of simple mono and binuclear metal carbonyls, metal nitrosyls, metal cyanides and dinitrogen complexes.

20. a) Write a note on carbonylation reactions.

    b) Write a note on asymmetric catalysis. Discuss asymmetric hydrogenation, isomerisation and epoxidation.

21. Discuss oxygen transport mechanism. What are the functions of haemoglobin and myoglobin in oxygen transport?

22. a) Discuss important analytical applications of radioisotopes.

    b) Outline fluxional isomerism of allyl, cyclopentadienyl and allene systems.

(2 x 5 = 10)

MSc Degree End Semester Examination

Semester I: Chemistry / Pharmaceutical Chemistry

21P1CHET02 / 21P1CPHT02 – BASIC ORGANIC CHEMISTRY

(2021 admission onwards)

Time: Three hours Max. Weight: 30

Section- A

(Answer any **eight** questions. Each question carries a weight of 1)

1. Explain inductive effect with suitable examples
2. What is meant by 1) chirality 2) diastereoisomers
3. What is meant by topicity? Explain by examples
4. Explain the mechanism of photo Fries rearrangement
5. Give the mathematical form of Hammet equation and explain the terms.
6. What is primary kinetic isotope effect?
7. What type of compounds are named by using the prefixes erythro and threo? Give one example.
8. What is Hammond postulate?
9. Draw the structure of the following molecules
    1. (2R, 3S)-2,3-dichloropentane
    2. S-1-bromo-1-chloropropane
10. Draw the conformations of cyclohexane derivatives.

(8 x 1 = 8)

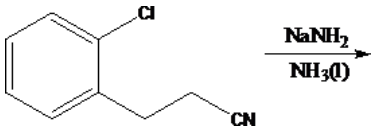
Section B

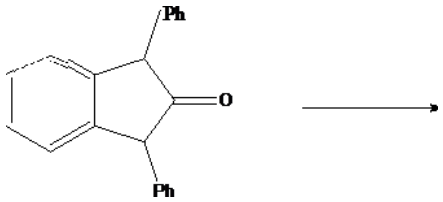
(Answer any **six** questions. Each question carries a weight of 2)

11.Predict the product and explain the mechanism

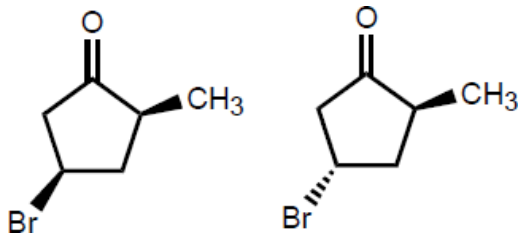
a)

b)





12. What are the applications of Taft equation in ester hydrolysis?
13. Write a note on Fullerenes and Graphene.
14. What are hard and soft acids? Use HSAB principle to distinguish them
15. Differentiate between kinetic and thermodynamic control of organic reactions.
16. Explain Curtin Hammett principle
17. Explain with example how NMR used to distinguish enantiotopic/ diastereotopic ligands.
18. Is it theoretically possible to separate the pair of compounds below by distillation? Explain briefly.



(**6 x 2 = 12**)

Section C

(Answer any **two** questions. Each question carries a weight of 5.)

19. a) Illustrate the conformational studies of i) Decalin ii) Adamanatane
    b)Explain the mechanism of semipinacolic deamination.
20. How do mesomeric ,hyperconjugative and steric effects influence the strength of organic bases ?
21. Explain the Nucleophilic substitution reactions in aromatic systems
22. Explain in detail about;
    a) Carbon based chiral centers.
    b) N based chiral centers.
    c) S based chiral centers.

(2 x 5 = 10)

MSc Degree End Semester Examination

Semester I: Chemistry / Pharmaceutical Chemistry

21P1CHET03 / 21P1CPHT03 – PHYSICAL CHEMISTRY - I

(2021 admission onwards)

Time: Three hours Max. Weight: 30

Section- A

(Answer any **eight** questions. Each question carries a weight of 1)

1. Explain the term fugacity. What is the physical significance of fugacity?
2. What are Maxwell relations? Explain.
3. Explain the term chemical potential? Derive the Gibbs-Duhem equation?
4. Define thermodynamic excess functions. Formulate expression for excess Gibbs free energy.
5. Define mean free path and collision frequency. How do they vary with pressure and temperature?
6. Explain the terms (a) phase space,(b)microstates, (c) macrostates
7. Derive the relation between thermodynamic probability and entropy.
8. Briefly explain the statistical formulations of third law of thermodynamics.
9. What is partition function ? How is it factorised into contributing parts ?
10. Distinguish between Bosons and Fermions**.**

(8 x 1 = 8)

Section B

(Answer any **six** questions. Each question carries a weight of 2)

11. What is meant by thermodynamics of mixing? Derive Gibbs-Duhem- Margules equation.
12. Derive Gibb's –Helmholtz equation. What are it's applications.
13. Derive Maxwell's law of distribution of velocities.
14. Explain Bose-Einstein condensation.
15. Derive Sackur – Tetrode equation applicable to monoatomic gases.
16. The free energy change ΔG accompanying a given process is -85.77 kJ at 25^{o}C and –83.68 kJ at 35^{o}C. Calculate the change in enthalpy (ΔH) for the process at 30^{o}C.
17. Calculate the translational entropy of gaseous iodine at 298K and 1 atm.
18. Calculate the rotational partiton function for hydrogen molecule at 300K. Moment of inertia of hydrogen molecule is 4.59×10^{-47}Kgm^2 symmetry number σ=2.

(**6 x 2 = 12**)

Section C

(Answer any **two** questions. Each question carries a weight of 5)

19. What is Nernst heat theorem? Explain the determination of absolute entropies using third law?

20. Discuss about a three component system taking suitable example and give its graphical representation.

21. (a) Derive an expression for Fermi-Dirac statistics (b) Give comparative account of the three statistics.

22. Derive Debye theory of heat capacity of solids. How does it differ from Einstein theory?

(2 x 5 = 10)

MSc Degree End Semester Examination

Semester I: Chemistry / Pharmaceutical Chemistry

21P1CHET04 / 21P1CPHT04 – QUANTUM CHEMISTRY AND GROUP THEORY

(2021 admission onwards)

Time: Three hours Max. Weight: 30

Section- A

(Answer any **eight** questions. Each question carries a weight of 1)

1. Predict the point group of (i) glyoxal (ii) cis-$[Co(en)_2Cl_2]^+$
2. Explain what are cyclic groups?
3. What are sub groups? How many sub groups are possible for D_3h?
4. List all the elements of benzene
5. Obtain the inverse of Sn^m,when n is even and m is even/odd
6. What are nodes? How many nodes are there in the plot of radial probability function for a 4p orbital?
7. Given below are the certain wave functions. State which of them are eigen function of d^2/dx^2. If so give the eigen values : a) A+B sin ax; (b) A cos ax (c) Ae^{ax}
8. Define recursion relation
9. What are Ladder operators?
10. Explain the term spherical harmonics.

(8 x 1 = 8)

Section B

(Answer any **six** questions. Each question carries a weight of 2)

11. Show that L^2 and L_y commute.
12. Show that the normalized wave function for a particle in a 3D box with sides of length a, b and c is $\Psi(x,y,z) = (8/abc)^{1/2}$ (sinnxΠx/a) (sinnyΠy/b)(sinnzΠz/c) and discuss the degeneracies of the first few energy levels.
13. Explain the postulate of spin by Uhlenbeck and Goudsmith, discovery of spin-Stern Gerlach experiment.
14. Derive an expression for wave equation of particle on a ring
15. Prepare GMT for (i) C_{2h} (ii) C_{3v}
16. Discuss screw axis and glide planes for crystals.
17. Derive the matrix for C_n and hence S_n element.
18. State and explain Great Orthogonality Theorem

(**6 x 2 = 12**)

Section C

(Answer any **two** questions. Each question carries a weight of 5.)

19. Construct the character table for C_3v and hence obtain the SALC.
20. Obtain the matrix representations for symmetry elements of NH_3
21. Explain 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
22. What are Hermite polynomials? How they are used for solving Schrödinger equation for a harmonic oscillator

(2 x 5 = 10)

MSc Degree End Semester Examination

Semester II: Chemistry / Pharmaceutical Chemistry

21P2CHET05 / 21P2CPHT05 – INORGANIC CHEMISTRY-II

(2021 admission onwards)

Time: Three hours Max. Weight: 30

Section- A

(Answer any **eight** questions. Each question carries a weight of 1)

1. What is chelate effect?
2. What is nephelauxetic effect?
3. Write the term symbol for a d1 configuration.
4. What are the demerits of Orgel diagrams?
5. Give an example for mixed outer and inner sphere reactions.
6. What do you mean by hard and soft ligands?
7. How do 4f orbitals differ from 5f orbitals?
8. Give two applications of organolanthanoid complexes in catalysis.
9. Give an example for the use of coordination compounds as catalysts in asymmetric synthesis.
10. Discuss effect of H+ on the rates of substitution of chelate complexes.

(8 x 1 = 8)

Section B

(Answer any **six** questions. Each question carries a weight of 2)

11. Write a note on the thermodynamic aspects of complex formation.
12. Discuss Jahn Teller effect.
13. Explain trans-effect theory for the substitution reactions in square planar complexes.
14. Sketch the Tanabe-Sugano diagram for [V(H2O)6]3+.
15. a) Discuss geometrical isomerism in octahedral complexes.
    b) Write a note on electronic and steric factors affecting linkage isomerism.
16. Compare the coordination chemistry of lanthanoids and actinoids with special reference to electronic spectra and magnetic properties.
17. Discuss inner sphere and outer sphere mechanisms of electron transfer reactions.
18. Give an account of qualitative treatment for the correlation diagram of d9 system.

(6 x 2 = 12)

Section C

(Answer any **two** questions. Each question carries a weight of 5)

19. Give an account of crystal field theory. Discuss splitting of d orbitals in octahedral, tetrahedral, square planar, square pyramidal and triagonal bipyramidal fields. List the drawbacks of crystal field theory.
20. Give an account of magnetic properties of complexes.
21. Write a note on optical isomerism in octahedral complexes. Describe resolution of optically active complexes and determination of absolute configuration of complexes by ORD and circular dichroism.
22. Give an account of kinetics and mechanism of substitution in octahedral complexes with special reference to dissociative and associative mechanisms, base hydrolysis and solvolytic reactions.

(2 x 5 = 10)

MSc Degree End Semester Examination

Semester II: Chemistry / Pharmaceutical Chemistry

21P2CHET06 / 21P2CPHT06 – ORGANIC REACTION MECHANISM

(2021 admission onwards)

Time: Three hours Max. Weight: 30

Section- A

(Answer any **eight** questions. Each question carries a weight of 1)

1. Give one example each for the insertion reaction and addition reaction of carbenes.
2. Distinguish between classical and non-classical carbocations
3. Briefly explain the Woodward Hoffmann rule
4. Write a note on oxymercuration
5. How can you obtain cycloheptanone from cyclohexanone
6. Discuss the regioselectivity of addition reactions with suitable examples.
7. What is Clemmenson reduction. Give mechanism
8. Write down the product and mechanism of the following reaction
9. Discuss Baldwin's rules.
10. What are Grignard reagents? Write down their applications? **(8 x 1 = 8)**

Section B

(Answer any **six** questions. Each question carries a weight of 2)

11. Discuss anti Markovnikov's addition mechanism
12. Identify the reaction and discuss the mechanism of the following reaction
13. Write a note on Mannich reaction
14. Use appropriate reagents and discuss the mechanism of the reaction
15. Give the mechanism and stereochemistry of Diels- Alder reaction
16. Write briefly on Lossen rearrangement
17. What are enolates. Compare them with enamines in synthetic applications
18. Discuss the mechanism of Stobbe condensation and its synthetic applications **(6 x 2 = 12)**

Section C

(Answer any **two** questions. Each question carries a weight of 5)

19. What are carbanions? Discuss their formation, structure and stability. What are their importances as reaction intermediates?
20. Give the mechanism of the following reactions.

1) Wolf rearrangement 2) Michael addition 3) Cannizaro reaction
4) Darzen condensation

21. What are the different types of pericyclic reactions? Discuss the importances of pericyclic reactions in organic synthesis.

22.

i.) How can you generate nitrenes?

ii.) Differentiate between SN1 and SN2 reactions.

iii.) Discuss the mechanism of halolactonisation.

(2 x 5 = 10)

MSc Degree End Semester Examination

Semester II: Chemistry / Pharmaceutical Chemistry

21P2CHET07 / 21P2CPHT07 – PHYSICAL CHEMISTRY-II

(2021 admission onwards)

Time: Three hours Max. Weight: 30

Section A

(Answer any **eight** questions. Each question carries a weight of **1**)

1. What is FID and FT in NMR spectroscopy?
2. What is Born Oppenheimer approximation? Explain the cases where the Born Oppenheimer approximation breaks down.
3. What is fermi resonance? Give one example.
4. Explain mutual exclusion principle**.**
5. Which of the following molecules exhibit pure rotational spectra? HF, NH_3, H_2O, CO, CH_4, BF_3, CO_2 , F_2.
6. Differentiate between first order and second order NMR spectra
7. What are fine structure and hyperfine structure in ESR spectrum?
8. What is Resonance Raman Spectrum?
9. What is finger print region in IR?
10. Discuss Frank condon principle. **(8 × 1 =8)**

Section B

(Answer any **six** questions. Each question carries a weight of 2)

11. Explain the basic principle of NQR spectroscopy.
12. Give the applications of ESR and Mossbauer methods in spectroscopy
13. Explain the terms chemical shift, coupling constant and factors influencing coupling constant in NMR spectroscopy
14. The first line in the rotational spectrum of NO appears at 1.72 cm^{-1} and its force constant is 1608 Nm^{-1}. Calculate the internuclear distance in A^0, vibrational frequency in cm^{-1} and energy in joules required for J = 3 to 4 rotational transition.
15. The first three vibrational energy of HCl were found to be at 2886, 5668 and 10923 cm^{-1}. Calculate the anharmonicity constant, zero point energy and the equilibrium oscillation frequency. Calculate the centrifugal distoration constant if the rotational constant is 21.18 cm^{-1} .
16. Discuss photoelectron spectroscopy.
17. Explain the various relaxation methods in NMR.

18. What is meant by normal mode of vibration? How many normal modes of vibration do the following molecules have? NH_3 , HCN , SO_2 **(6 × 2 = 12)**

Section C

(Answer any two questions. Each question carries a weight of 5)

19. Explain the following in NMR spectroscopy
    a) Larmor Precision
    b) Chemical shift and its representation
    c) Magic angle spinning
20. Explain the classical theory of Raman spectroscopy.
21. Discuss the theory and applications of NQR Spectroscopy.
22. Write note on:
    a) Resonance fluorescence
    b) Predissociation
    c) Mechanism of Laser action
    d) Polarized and depolarized Raman lines **(5 × 2 = 10)**

MSc Degree End Semester Examination

Semester II: Chemistry / Pharmaceutical Chemistry

21P2CHET08 / 21P2CPHT08 – THEORETICAL AND COMPUTATIONAL CHEMISTRY

(2021 admission onwards)

Time: Three hours Max. Weight: 30

Section A

(Answer any **eight** questions. Each question carries a weight of 1)

1. What are slater determinants?
2. State and Explain Variation theorem
3. State and explain Non crossing rule in quantum mechanics
4. Explain Hellmann-Feynmann theorem.
5. Find out the characters for all the symmetry operations of NH_3 molecule using Cartesian coordinates.
6. What are the group theoretical selection rules for an electronic transition to be allowed?
7. Explain AMBER.
8. What is CHARMM? Explain its use in molecular mechanics.
9. What is Koopman's Theorem?
10. Write a short note on Independent Electron Approximation **(8 x 1 = 8)**

Section B

(Answer any **six** questions. Each question carries a weight of 2)

11. Illustrate variation theorem using the trial wave function x(a-x) for particle in a one dimensional box
12. Explain Huckel molecular orbital theory of Butadiene and Benzene
13. Explain how group theory helps to predict optical activity
14. Using Direct Product Tables, predict the electronic transitions of C_2v and C_3v molecules.
15. What are the important assumptions used in HFSCF method?
16. Explain how to build a Z-matrix?
17. Compare MOT and VBT
18. Explain the Kohn-Sham approach used in DFT? **(6 x 2 = 12)**

Section C

(Answer any **two** questions. Each question carries a weight of 5)

19. How GAMESS is input file prepared? Illustrate with reference to water molecule?

20. Using group theory, derive the allowed electronic transitions in formaldehyde.
21. Explain Perturbation Method? Illustrate with Helium as Example
22. Explain molecular orbital theory and derive an expression for energy and wave function of Hydrogen molecule. **(2 x 5 =10)**

MSc Degree End Semester Examination

Semester III: Pharmaceutical Chemistry

21P3CPHT09 – DRUG DESIGN AND PHARMACOLOGY

(2021 admission onwards)

Time: Three Hours Max. Weight: 30

Section- A

(Answer any **eight** questions. Each question carries a weight of 1)

1. What to do you mean by G-Coupled receptors?
2. Explain Pharmacophere
3. Discuss any one receptor theory
4. What is LD50?
5. What is the pharmacological action of Nystatin and Ribavirin?
6. Give the structure of sulfamethoxole and pyrimethamine
7. What are Antiarrhythmic Drugs?
8. Draw the structure of verapamil and Fluvastatin
9. What do you mean by first line and second line drugs?
10. What are anti gout drugs?

(8 x 1 = 8)

Section B

(Answer any **six** questions. Each question carries a weight of 2)

11. Explain in detail the mechanism of action of Anti Amoebic and Antihelmintics.
12. Write a note on antiviral agents.
13. Discuss the pharmacological action of a) Digitoxin, b) Methyldopa, c) Nifedipine and d) Lovastatin
14. Explain in detail about Anti-coagulants
15. Outline the synthesis of a) Streptomycin and b) Isoniazid.
16. Discuss chemotherapy of malaria.
17. Explain SAR of Phenyl ethyl piperidines used as analgesics
18. Write a note on COX I and COX II inhibitors.

(6 x 2 = 12)

Section C

(Answer any **two** questions. Each question carries a weight of 5)

19. Illustrate the different pharmacokinetic principles employed in pharmacology
20. Explain in detail Biotransformation of drugs. Account for Phase I and Phase II reactions
21. Describe in detail the classification of antibiotics, mechanism of action and therapeutic uses
22. What are antipyretics and NSAIDs? Discuss in detail the classification of compounds used as antipyretics and NSAIDs.

MSc Degree End Semester Examination

Semester III: Chemistry / Pharmaceutical Chemistry

21P3CHET10 / 21P3CPHT10 – ORGANIC SYNTHESES

(*2021 admission onwards*)

Time: 3 Hours Max. Weight: 30

Section- A

(Answer any **eight** questions. Each question carries a weight of 1)

1. What are the important uses of (1)DDQ and (2)DCC
2. Define Pauson-Khand reaction with example
3. Give one application of Baker's yeast in organic synthesis
4. Give the importance of amino protection in peptide synthesis
5. What is Passerini reaction? Give its mechanism
6. Give an example for Huisgen 1,3-dipolar addition
7. Give one example for ring closing metathesis using Grubb's catalyst.
8. How oxetanes can be produced photochemically? Explain with example
9. Describe Shi epoxidation? What are its applications?
10. Give an example for Sarrett oxidation with example?

(8 x 1 = 8)

Section B

(Answer any **six** questions. Each question carries a weight of 2)

11. Explain how Wilkinson's catalyst and Nickel catalyst helps in catalytic hydrogenation ,starting its mechanism of action
12. Explain the following reactions using suitable examples: (a) Nef reaction (b) Tishchenko reaction
13. Give the synthetic utility of Gilmann reagent in organic synthesis
14. Write notes on (a) Cation –Olefin cyclization(b) Radical –Olefin cyclization
15. Briefly explain the retrosynthesis of D-luciferin
16. Discuss the synthetic utility of trialkylstannane in organic synthesis.
17. Explain the mechanism of the following reactions(a) Brook rearrangement(b) Ireland-Claisen rearrangement
18. Discuss the relevant protecting groups used in Peptide synthesis with examples

(6 x 2 = 12)

Section C

(Answer any **two** questions. Each question carries a weight of 5.)

19. Give an account of the chemoselectivity in metal hydride reductions with special references to (1) $NaCNBH_3$ (2) DIBAL-H (3) Red-Al (4) LiAlH4
20. How are the following heterocyclic compounds synthesized?
    (a) Oxazole (b) Imidazole (c) Thiophene (d) Pyrrole
21. Describe the synthetic utility of the following reactions:
    (a) Moffatt –Pfitzner oxidation
    (b) Hydroboration
    (c) Sarrett oxidation
    (d) TebbeOlefination
22. Write notes on the metal mediated C-C and C-X coupling reactions coupling reactions with special reference to :
    (a) Suzuki-Miyaura coupling
    (b) Sonogashira coupling
    (c) Heck coupling
    (d) Glaser coupling (**2 x 5 = 10**)

MSc Degree End Semester Examination

Semester III: Chemistry / Pharmaceutical Chemistry

21P3CHET11 / 21P3CPHT11 – PHYSICAL CHEMISTRY-III

(*2021 admission onwards*)

Time: 3 Hours Max. Weight: 30

Section A

(Answer any **eight** questions. Each question carries a weight of 1)

1. What do you mean by branching chain reactions?
2. Distinguish between general and specific H+ ion catalysis
3. What is structure factor? Explain its significance.
4. Define reciprocal lattice. What is its significance?
5. What are Miller Indices? How are they determined?
6. What is potential energy surface? Explain its significance.
7. Define Zeta potential.
8. What are oscillating chemical reactions? Give one example.
9. Explain the principle of SEM.
10. What is steady state approximation? **(8 × 1 = 8)**

Section B

(Answer any **six** questions. Each question carries a weight of 2)

BUNCH 1 (Short Essay Type)

11. Explain the principle of Surface Enhanced Raman Spectroscopy.
12. Explain the Rice Herzfeld mechanism of organic decomposition reactions of acetaldehyde with special reference to Gold finger, Niclause and Letort rule.
13. Explain the Lotka- Volterra mechanism of oscillating chemical reactions.
14. Briefly describe the methods of characterising crystal structure.

BUNCH 2 (Problem Type)

15. 150 ml of N_2 (1atm pressure at 0 ^{0}C) was required to form a monolayer on the surface of silica gel. Calculate the surface area of the solid. The cross-sectional area of N_2 is 0.162 $(nm)^2$.
16. For the first order isomerisation of an organic compound at 130 ^{0}C, the activation energy is 108.4 KJ/mol and the specific reaction rate is 9.12×10^{-4} sec^{-1}. Calculate the standard entropy of activation and standard enthalpy of activation.

17. The enzyme catalysed conversion of a substance at 25^{o}C has a Michealis constant of 0.042 mol L^{-1}. The rate of reaction is 2.45 mol L^{-1} s^{-1} when the substrate concentration is 0.890 mol L^{-1}. What is the maximum velocity of the enzymolysis?

18. For a homogeneous reaction the rate constants are 3.0 x 10^{-5} Lmol s^{-1} and 1.2 x 10^{-3} L mol s^{-1} at 629 K and & 00 K respectively. Calculate the energy of activation and frequency parameter.

(6 × 2 = 12)

Section C

(Answer any **two** questions. Each question carries a weight of 5)

19. (a) Describe how the limitations of Lindemann theory of unimolecular reaction is overcome by Hinshelwood and RRK modification.

    (b) Compare transition state theory with collision theory.

20. (a) Explain the rotating crystal method for the X-ray diffraction studies of crystals.

    (b) Explain the Eley-Rideal mechanism for the bimolecular reaction on the surface of solids.

21. Derive the BET adsorption isotherm. Show that it approximates to Langmuir adsorption isotherm under limiting conditions.

22. Describe the Semenov-Hinshelwood theory of branching chain reaction. Explain the lower and upper explosion limits with respect to the kinetic expression.

(2 × 5 = 10)

MSc Degree End Semester Examination

Semester III: Chemistry / Pharmaceutical Chemistry

21P3CHET12 / 21P3CPHT12 – SPECTROSCOPIC METHODS IN CHEMISTRY

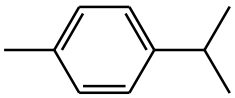
(*2021 admission onwards*)

Time: 3 Hours Max. Weight: 30

Section- A

(Answer any **eight** questions. Each question carries a weight of 1)

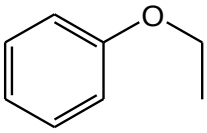
1. Calculate the λ_{max} for the compound.



2. Which of the following isomers of pentadiene will show the largest wavelength of UV absorption? Give reason.

   i) CH_2=CH-CH=CH-CH_3 ii) CH_2=CH-CH_2-CH=CH_2

3. 2-Hydroxy-3-nitroacetophenone shows two carbonyl stretching frequencies at 1692 and 1658 cm^{-1}. Explain.
4. C-H stretching frequency increases from alkane → alkene → alkyne. Explain.
5. Show the formation of the peak at m/z = 94 in the mass spectrum of



6. Predict the number of signals and sketch the NMR spectrum of CH_3-O-CH_2-CH_2-Cl.
7. What are shift reagents in NMR spectroscopy? Explain.
8. How NMR spectroscopy is useful in distinguishing cis-stilbene and trans-stilbene?
9. Explain off resonance decoupling.
10. Explain the spin notation A_2X_3 in NMR spectroscopy with example.

(8 × 1 =8)

Section B

(Answer any **six** questions. Each question carries a weight of 2)

11. Explain the exchange phenomenon in ^{1}H NMR.
12. Discuss the effect of concentration on vibrational stretching frequency of methyl salicylate and ethanol.
13. A compound with molecular formula $C_4H_8O_3$ gave the following spectral data. Deduce the structure.

    IR: 1120, 1705 cm^{-1}

1H NMR: δ 12.1(1H, s), 4.15(2H, s), 3.6(2H, q, J = 7 Hz) and 1.3(3H, t, J = 7 Hz) ppm

14. Write a note on HRMS and MS-MS.
15. Explain McLafferty rearrangement.
16. Discuss the technique - spectral editing based on DEPT.
17. Briefly explain cross polarization and selective population inversion in NMR spectroscopy.
18. A compound 'A' with molecular formula C_5H_{10} on ozonolysis gives 'B', C_4H_8O, as one of the products. The IR spectrum of B showed a band at 1720 cm^{-1} and the NMR spectrum showed three signals at δ values 0.9 (3H, t), 3.4 (2H, q) and 2.2 (3H, s). What are A and B? Explain.

(6 × 2 = 12)

Section C

(Answer any **two** questions. Each question carries a weight of 5)

19. Describe the following

    a) FAB b) MALDI c) Field desorption d) TOF e) Cyclotron

20. Predict the structure of the compound (MF $C_{11}H_{20}O_4$) which gave the following spectral data.

    UV – No λ_{max} above 200 nm IR: 1740 cm^{-1}.

    1HNMR: δ 4.2 (4H, q), 3.3 (1H, t), 1.9 (2H, q), 1.33 (4H, m), 1.27 (6H, t) and 0.9 (3H,t) ppm.

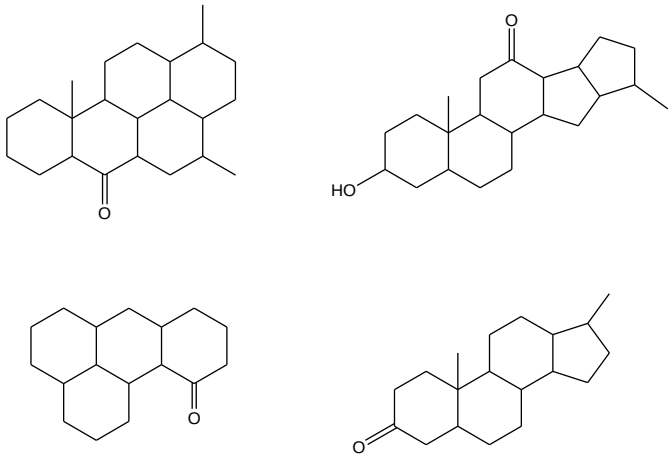
    13C NMR: δ 14.10, 13.81, 22.4, 28.5, 29.5, 52.0, 61.1 and 169.3 ppm.

    Mass: m/z 216 ($M^{+\cdot}$), 171, 160 (100%), 133 and 115.

21. (a). Explain the magnetic anisotropy in carbonyl compounds and acetylene.

    (b). Define spin – spin coupling. Explain spin-spin coupling in the spin systems AX_2, AMX and ABC with examples.

22. Discuss Octant rule. Draw the octants for the following compounds and predict the sign of their optical activity.



MSc Degree End Semester Examination

Semester IV: Pharmaceutical Chemistry

21P4CPHT13EL – BIOCHEMISTRY AND BACTERIOLOGY

(*2021 admission onwards*)

Time: 3 Hours Max. Weight: 30

Section A

(Answer any **eight** questions. Each question carries a weight of 1**)**

1. Discuss the relevance of sucrose in pharmaceutical chemistry.
2. Explain the structure of cell membrane.
3. What are the advantages of Solid Phase Peptide Synthesis (SPPS) over Solution Phase Synthesis (SPS)? Give an example for a solid support used in SPPS.
4. Explain the role of Boc and DCC in the Merrifield pep□de synthesis.
5. Briefly explain recombinant technology in enzyme synthesis?
6. Explain the role of aspirin as an inhibitor for PGH2 synthase?
7. What are the functions of adreno cortico trophic hormones?
8. What is restriction enzyme? What is its biological significance?
9. Explain the role of Coenzyme A on biosynthesis of fatty acids.
10. What do you mean by staining of bacteria?

(8 x 1 = 8)

Section B

(Answer any **six** questions. Each question carries a weight of 2**)**

11. Explain the different chromatographic technics used in the amino acid analysis.
12. Explain Ramachandran plot.
13. Write a note on classification of enzymes? Explain the mechanism of ac□on?
14. What is allosteric inhibition? Explain the mechanism citing suitable examples.
15. Give the structure and functions of adrenal cortical hormones.
16. What are the functions of neurohypophysis?
17. Describe the biogenesis of prostaglandins.
18. Discuss fructose metabolism.

(6 x 2 = 12)

Section C

(Answer any **two** questions. Each question carries a weight of 5**)**

19. Discuss clinical use of enzymes and enzyme immobilization? Explain enzyme linked immunosorbent assay?
20. Outline the synthesis of purine and pyrimidine nucleotides
21. Explain Hexose Monophosphate (HMP) Shunt.
22. Explain in detail about
    a) Different stages involved in the bacterial growth,
    b) Different processes involved in the control of microbial growth. **(2 x 5 = 10)**

MSc Degree End Semester Examination

Semester IV: Pharmaceutical Chemistry

21P4CPHT14EL – ADVANCES IN PHARMACEUTICAL OPERATIONS

(*2021 admission onwards*)

Time: 3 Hours Max. Weight: 30

Section A

(Answer any **eight** questions. Each question carries a weight of 1**)**

1. What is the effect of pH on the dissolution rate?
2. Give the uses of Iodine -131 as a radiopharmaceutical
3. What is SPET?
4. What is the base for suppository? Give an example
5. Explain one advantage of tablets being enteric coated?
6. What are the entitlement of a work to copyright?
7. What do you mean by double blind study in clinical trials?
8. What are the types of suspension?
9. Explain the principle of separation of different components by liquid chromatography?
10. What is the effect of using solvent mixtures of different compositions in LC?

(8 x 1 = 8)

Section B

(Answer any **six** questions. Each question carries a weight of 2**)**

11. Give an account of the effect of drug solubility and particle size on drug dissolution.
12. Give an account of the chemical modifications used for increasing the solubility of a drug?
13. Explain the process of drying and sugar coating of tablets.
14. Explain the factors to improve physical stability of emulsions?
15. Write a note on properties of colloids?
16. Explain the preparation of an o/w and w/o emulsion
17. Explain any one parenteral dosage forms.
18. How is a nanoparticle drug delivery system designed?

(6 x 2 = 12)

Section C

(Answer any **two** questions. Each question carries a weight of 5**)**

19. Describe the working of counter current extractor and multiple evaporator.
20. Discuss the process and technique for the manufacture of tablet?
21. Explain briefly about complete specification of a patent.
22. a) Give the principle and working of a GCMS. What is the advantage of GCMS over GC? What are the applications in Pharmaceutical Industry?
    b) Explain the principle of separation and the applications of gel electrophoresis.

(2 x 5 = 10)

MSc Degree End Semester Examination

Semester IV: Pharmaceutical Chemistry

21P4CPHT15EL – MEDICINAL CHEMISTRY

(*2021 admission onwards*)

Time: 3 Hours Max. Weight: 30

Section A

(Answer any **eight** questions. Each question carries a weight of 1**)**

1. Define a lead compound.
2. Explain the method of linear regression analysis by least square method used in QSAR.
3. Describe Hammet equation. Explain the significance of the terms invovled.
4. Give an idea about the drug receptor interactions.
5. Give examples for non-bead form supports in solid phase synthesis.
6. What are traceless anchors?
7. What are antimetabolites? Give different types of antimetabolites.
8. Suggest a synthetic route for Tamoxifen.
9. What is the major reason for Alzheimer's disease?
10. What are anxiolytic agents? Give two examples.

(8 x 1 = 8)

Section B

(Answer any **six** questions. Each question carries a weight of 2**)**

11. Illustrate various applications of prodrugs with suitable examples.
12. Explain the concept of functional group modification to increase the potency of a drug.
13. List out the advantages and disadvantages of QSAR
14. What are the statistical methods commonly used in QSAR?
15. Write briefly on PEG-grafted polystyrene as solid support in solid phase synthesis.
16. Write briefly on different amino and carboxyl protecting groups.
17. Give an account of ergot alkaloids
18. Explain the synthesis and mechanism of action of barbiturates.

(6 x 2 = 12)

Section C

(Answer any **two** questions. Each question carries a weight of 5**)**

19. Write short note on drug-likeness screening.
20. Give an account of the alkylating agents in cancer chemotherapy.
21. Give the structure, mechanism of action and synthesis of salbutamol, methoxamine and Phentolamine
22. Write short note on the mechanism behind the action of hypnotics and sedatives.

(2 x 5 = 10)