KANNUR UNIVERSITY

(Abstract)

M.Sc Chemistry with Drug Chemistry Specialization programme- Scheme, Syllabus and Pattern of Question Papers (First and Second Semesters only) under Choice Based Credit and Semester System (in Outcome Based Education System-OBE) in Affiliated Colleges- Implemented with effect from 2023 Admission- Orders issued.

ACADEMIC C SECTION

ACAD C/ACAD C5/20041/2023 Dated: 04.10.2023

Read:-1. U.O No. Acad C2/429/2017 Dated 08.09.2020.

2. U. O No. Acad C1/21246/2019 Dated 07.12.2020.

3. U.O. No. Acad/C1/21246/2019 Dated 16.02.2023.

4. U.O. No. Acad/C1/21246/2019 Dated 20.04.2023.

5. Minutes of the meeting of the CSMC & Conveners of Adhoc committee held on 15.06.2023

6. Orders of the Vice Chancellor in the file No. Acad C1/21246/2019 Dated 05.08.2023.

7. U.O. No. Acad/C1/21246/2019 Dated 09.08.2023.

8. The Minutes of the meeting of the Ad hoc Committee for Chemistry (PG) held on 21.09.2023.

9. Syllabus of first and second semesters M.Sc Chemistry with Drug Chemistry Specialization programme submitted by the Convenor, Ad hoc Committee for Chemistry vide e-mail dated 23.09.2023

ORDER

1. A Curriculum Syllabus Monitoring Committee comprising the members of Syndicate was constituted for the Syllabus revision of U G & PG Programmes in Affiliated Colleges, vide paper read (1) above and as per the recommendation of this Committee in its meeting held on 20.11.2020, constitute a sub Committee to prepare the Regulation for PG programmes in Affiliated Colleges vide paper read (2) above.

2. As the reconstitution of Board of Studies of the University is under the consideration of the Hon'ble Chancellor, and considering the exigency of the matter, Ad hoc Committees were constituted vide paper read (3) above and it has been modified vide paper read (4) above, to revise the Curriculum and Syllabus of PG Programmes in Affiliated Colleges w.e.f 2023-24 academic year,.

3. The combined meeting of the Curriculum Syllabus Monitoring Committee & Conveners of Ad hoc committee held on 15.06.2023 at syndicate room discussed in detail the draft Regulation, prepared by the Curriculum Syllabus Monitoring Committee, for the PG programmes under Choice Based Credit and Semester System to be implemented in Affiliated Colleges w.e.f 2023 admission and proposed the different phases of Syllabus revision process such as subject wise workshop, vide the paper read (5) above.

4. The revised Regulations for Post Graduate Programmes under Choice Based Credit and Semester System (In OBE- Out Come Based Education System) was approved by the Vice-chancellor on 05.08.2023 and implemented w.e.f 2023 Admission vide Paper read (7) above.

5. Subsequently, as per the paper read (8) above, the Ad hoc Committee for Chemistry (PG)

finalized the Scheme, Syllabus and Pattern of Question Papers (1st & IInd Semesters) of M.Sc Chemistry with Drug Chemistry Specialization programme to be implemented with effect from 2023 Admission

6. As per the paper read (9) above, the Convener, Ad hoc Committee for Chemistry (PG) programme submitted the finalized copy of Scheme, Syllabus and Pattern of Question Papers (1st & IInd Semesters) of M.Sc Chemistry with Drug Chemistry Specialization programme for implementation with effect from 2023 Admission.

7. The Vice Chancellor after considering the matter in detail and in exercise of the powers of the Academic Council conferred under section 11(1) Chapter III of Kannur University Act, 1996 and all other enabling provisions read together with ***accorded sanction to implement the Scheme,*** **Syllabus and Pattern of Question Papers (1st & IInd Semesters) of M.Sc Chemistry with Drug Chemistry Specialization programme** ***under Choice Based Credit and Semester System (in OBE- Outcome Based Education System) in Affiliated Colleges under the University with effect from 2023 Admission***, subject to report to the Academic Council.

8. The Scheme, Syllabus and Pattern of Question Papers (1st & IInd Semesters) of M.Sc Chemistry with Drug Chemistry Specialization programme under Choice Based Credit and Semester System (in OBE- Outcome Based Education System) in Affiliated Colleges under the University with effect from 2023 Admission is uploaded in the University website.

9. Orders are issued accordingly.

Sd/-

Narayanadas K

DEPUTY REGISTRAR (ACAD)

For REGISTRAR

To:
1. Principals of Affiliated Colleges offering M.Sc Chemistry with Drug Chemistry Specialization programme
2. Convenor, Curriculum Syllabus Monitoring Committee.
3. Convenor, Ad hoc Committee for Chemistry (PG) programme.

Copy To:
1. The Examination Branch (Through PA to CE)
2. PS to VC / PA to PVC / PA to R/PA to FO
3. DR / AR 1 (Acad) /Computer Programmer
4. Web Manager (for uploading on the website).
5. EG 1/EX C1 (Exam), EP V
6. SF/DF/FC

Forwarded / By Order

SECTION OFFICER

KANNUR UNIVERSITY * THAVAKKARA * CIVIL STATION P.O. KANNUR Pin-670 002

KANNUR UNIVERSITY

(Abstract)

M.Sc. Chemistry with Drug Chemistry Specialization programme- Modified Scheme , Syllabus, Pattern of Question paper and Model Question Paper-Third and Fourth semester only - under Choice Based Credit and Semester System-(in OBE) in Affiliated Colleges-Implemented with effect from 2023 admissions- Orders issued

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ACADEMIC C SECTION

ACAD C/ACAD C5/20041/2023 Dated: 29.08.2024

Read:-1. U.O.No. ACAD C/ACAD C5/20041/2023 dtd: 04.10.2023

2. Minutes of the meeting of the BoS in Chemistry (PG) held on 22/05/2024

3. E-mail dtd 19/06/2024 from the Chairperson, BoS in Chemistry (PG)

4. The Minutes of the meeting of the Academic Council held on 25/06/2024

ORDER

1. The Scheme, Syllabus, Pattern of Question Papers and Model question papers of First & Second Semesters of the M.Sc.Chemistry with Drug Chemistry Specialization programme under CBCSS (In Outcome Based Education system) in Affiliated Colleges were approved and implemented with effect from 2023 admission, vide paper read (1) above.

2.Thereafter, the meeting of the Board of Studies in Chemistry (PG) held on 22.05.2024, vide paper read (2) discussed and finalized the Syllabuses of the third and fourth Semesters of the M.Sc. Chemistry with Drug Chemistry Specialization programme in affiliated Colleges w.e.f.2023 admission. The BoS (Board of Studies) recommended to change the IV Semester scheme as per the approved Regulations. As per the Clause 6.1 of the Regulations, the Scheme of Evaluation of each Courses contain two parts, viz a) Continuous Evaluation (CE) and End Semester Evaluation (ESE). 20% weightage shall be given to CE and 80% weightage shall be for the End Semester Evaluation. Therefore, the BoS modified the marks of MSCHD03 & 04 C18 (Industrial Visit/Institutional Visit/Internship) to 20:5 instead of 30:5 and MSCHD04C20 Viva Voce to 40:10, instead of 40 as ESE and thereby corrected the total marks distribution in IV Semester as 360:90, instead of 370:80.

3. Accordingly, the Chairperson, BoS in Chemistry (PG) submitted the Scheme (Modified) Syllabus, Pattern of Question paper and Model Question paper of M.Sc.Chemistry with Drug Chemistry specialization programme (Third and Fourth semesters) in Affiliated Colleges for implementing w.e.f.2023 admission vide paper read (3) above.

4.The Vice Chancellor after considering the matter in detail, ordered to place the same, before Academic Council for approval.

5. The XXVIII th Meeting of the Academic Council held on 25/06/2024 considered the matter and approved the Modified Scheme, Syllabus, Pattern of Question Papers and Model question papers of MSc Chemistry with Drug Chemistry specialization programme (Third and Fourth Semester) to be implemented in affiliated college w.e.f 2023 admission in principle and permitted to publish the same considering the urgency of the matter.

6.The Minutes of the Academic council has been approved and published.

7.The Modified Scheme, Syllabus, Pattern of Question Paper and Model Question Papers of 3rd &

4th semester M.Sc.Chemistry with Drug Chemistry specialization programme under Choice Based Credit and Semester System (in Outcome Based Education System) in Affiliated Colleges under the University with effect from 2023 Admission is appended with this U.O. and uploaded in the University website (www.kannuruniversity.ac.in).

Orders are issued accordingly.

Sd/-

ANIL CHANDRAN R

DEPUTY REGISTRAR (ACADEMIC)

For REGISTRAR

To: 1. Principals of Affiliated Colleges Offering M.Sc.Chemistry with Drug Chemistry Specialization programme

2. Chairperson, BoS , Chemistry (PG)

Copy To: 1. The Examination branch (Through PA to CE)

2. PS to VC/PA to R/Chairperson, BoS in Chemistry (PG)
3. DR/AR II (Acad) /Computer Programmer
4. Web Manager (for uploading on the website)
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Forwarded / By Order

SECTION OFFICER

KV

KANNUR UNIVERSITY
CIVIL STATION P.O.
KANNUR
Pin-670 002
THAVAKKARA

KANNUR UNIVERSITY

SYLLABUS

For MSc Programme in

CHEMISTRY WITH DRUG CHEMISTRY SPECIALIZATION in affiliated colleges-2023

Syllabus under Choice Based Credit and Semester System with effect from 2023 admission

OUTCOME-BASED EDUCATION - SYSTEM (OBE)

2023

INDEX

1. PREFACE

The syllabi of the MSc programme in Chemistry with Drug Chemistry Specialization offered in the university's affiliated colleges under the semester system were revised in light of the decision of the Syndicate of Kannur University, Curriculum Syllabus Monitoring Committee, PG Board of Studies and Chemistry (PG) Ad hoc committee meetings, and the revised syllabi are effective from 2023 admission onwards. There are two independent PG programmes in Chemistry for affiliated colleges, namely MSc Chemistry, and M Sc Chemistry with Drug Chemistry Specialization. The ad-hoc committee formed by Kannur University as per order number Acad/C1/21246/2019 dated 10/02/2023, Kannur University, has prepared the revised curriculum and syllabus for both the programmes to be outcome-based by 2023 regulations.

Candidates with bachelor's degrees in Chemistry/Polymer Chemistry with Mathematics and Physics/Computer science as subsidiary subjects are eligible for admission to these courses. Rules regarding minimum marks required for the Bachelor's degree, reservation, etc., will be as laid down by the University from time to time. The coursework shall be by the scheme of valuation and syllabus prescribed.

POST-GRADUATE PROGRAMME IN CHEMISTRY WITH DRUG CHEMISTRY SPECIALIZATION

(Syllabus under choice credit-based semester system (OBE) with effect from 2023 admission)

Master of Science in Chemistry with Drug Chemistry specialization is a postgraduate level course that aims at an advanced level understanding of major concepts, theoretical principles, experimental aspects, and research aptitudes in chemical sciences with special references to drug chemistry. The MSc Chemistry program is designed to provide students with advanced knowledge and skills in various branches of chemistry. Following the principles of Outcome-Based Education (OBE), the program aims to equip students with the necessary theoretical foundation, practical laboratory skills, and critical thinking abilities required for successful careers in academia, industry, or research.

The MSc program consists of a comprehensive curriculum that includes a combination of core courses, elective courses, laboratory work, Industrial/Institutional visits, internships, and a research project. The program allows students to specialize in specific areas of chemistry based on their interests and career aspirations. The course consists of four theory papers each and three practical papers in the 1st and IInd semesters. There will be three theory papers, one

open/multi-disciplinary elective paper, and three practical papers (to be continued in semester IV) in the IIIrd semester. Two elective papers, three practical papers, a project, an industrial/institutional visit/ internship along with a general viva voce will be there in the IVth semester. The students may select one elective paper from each of the elective groups. Each theory paper and elective paper is of 3 hours duration and each practical paper is of 6 hours duration. The total marks for the entire course shall be 1500 and the total credit shall be 80. 20% of marks shall be allocated for internal assessment of theory and practical papers each. The PG programme shall extend over a period of two academic years comprising four semesters, each of 450 hours in 18 weeks duration.

The program utilizes continuous assessment methods to measure and evaluate student learning outcomes. These assessments may include examinations, laboratory reports, research papers, presentations, and project work. Feedback and constructive criticism are provided to facilitate student growth and improvement.

Graduates of the MSc Chemistry with Drug Chemistry Specialization program will be well-prepared for diverse career paths. They can pursue employment opportunities in research and development laboratories, pharmaceutical and chemical industries, government agencies, educational institutions, and more. The program also lays a strong foundation for those interested in pursuing further studies and research at the doctoral level.

The MSc Chemistry with Drug Chemistry Specialization program, aligned with Outcome-Based Education, offers students a comprehensive education in chemistry and prepares them for successful careers in the field. By focusing on defined outcomes and emphasizing practical skills, critical thinking, and research abilities, the program ensures that students are well-equipped to address the challenges and contribute to advancements in the field of chemistry.

2. VISION AND MISSION STATEMENTS

Vision:

To establish a teaching, residential, and affiliating University and to provide equitable and just access to quality higher education involving the generation, dissemination, and critical application of knowledge with a special focus on the development of higher education in Kasaragod and Kannur Revenue Districts and the Manantavady Taluk of Wayanad Revenue District.

Mission:

➢ To produce and disseminate new knowledge and to find novel avenues for the application of such knowledge.

➢ To adopt critical pedagogic practices which uphold scientific temper, the uncompromised spirit of inquiry, and the right to dissent.

➢ To uphold democratic, multicultural, secular, environmental, and gender-sensitive values as the foundational principles of higher education and to cater to the modern notions of equity, social justice, and merit in all educational endeavours.

➢ To affiliate colleges and other institutions of higher learning and to monitor academic, ethical, administrative, and infrastructural standards in such institutions.

➢ To build stronger community networks based on the values and principles of higher education and to ensure the region's intellectual integration with national vision and international standards.

➢ To associate with the local self-governing bodies and other statutory as well as non-governmental organizations for continuing education and also for building public awareness on important social, cultural, and other policy issues.

3. THE PROGRAMME OUTCOMES (POs)

Programme Outcomes (POs): Programme outcomes can be defined as the objectives achieved at the end of any specialization or discipline. These attributes are mapped while a student is doing graduation and determined when they get a degree.

PO 1. Advanced Knowledge and Skills: Postgraduate courses aim to provide students with in-depth knowledge and advanced skills related to their chosen field. The best outcome would be to acquire a comprehensive understanding of the subject matter and develop specialized expertise.

PO 2. Research and Analytical Abilities: Postgraduate programs often emphasize research and analytical thinking. The ability to conduct independent research, analyze complex problems, and propose innovative solutions is highly valued.

PO 3. Critical Thinking and Problem-Solving Skills: Developing critical thinking skills is crucial for postgraduate students. Being able to evaluate information critically, identify patterns, and solve problems creatively are important outcomes of these programs.

PO 4. Effective Communication Skills: Strong communication skills, both written and verbal, are essential in various professional settings. Postgraduate programs should focus on enhancing communication abilities to effectively convey ideas, present research findings, and engage in academic discussions.

PO 5. Ethical and Professional Standards: Graduates should uphold ethical and professional standards relevant to their field. Understanding and adhering to professional ethics and practices are important outcomes of postgraduate education.

PO 6. Career Readiness: Postgraduate programs should equip students with the necessary skills and knowledge to succeed in their chosen careers. This includes practical skills, industry-specific knowledge, and an understanding of the job market and its requirements.

PO 7. Networking and Collaboration: Building a professional network and collaborating with peers and experts in the field are valuable outcomes. These connections can lead to opportunities for research collaborations, internships, and employment prospects.

PO 8. Lifelong Learning: Postgraduate education should instil a passion for lifelong learning. The ability to adapt to new developments in the field, pursue further education, and stay updated with emerging trends is a desirable outcome.

4. PROGRAMME SPECIFIC OUTCOMES OF MSc CHEMISTRY WITH DRUG CHEMISTRY SPECIALIZATION

Program Specific Outcomes (PSOs) serve as a framework to outline the specific goals and expected learning outcomes of the MSc Chemistry program. These outcomes are designed to ensure that graduates possess the necessary knowledge, skills, and abilities to excel in their careers or pursue further research in the field of chemistry. The Programme Specific Outcomes are given below.

PSO 1. In-depth knowledge of core concepts: Understanding of the fundamental principles and theories in various sub-disciplines of chemistry, including organic, inorganic, physical,

analytical, theoretical, and drug chemistry.

PSO 2. Advanced laboratory skills: Possess advanced laboratory skills necessary for planning, executing, and analyzing experiments in diverse areas of chemistry. This includes skill in handling chemical reagents, instruments, and equipment, as well as accurate measurement techniques.

PSO 3. Research and scientific inquiry: Exhibit competence in designing and conducting independent research projects related to new chemical entities and developing synthetic strategies and drug design proposals, including formulation of research questions, implementing methodologies, collecting and interpreting data, and drawing appropriate conclusions.

PSO 4. Critical thinking, data analysis, interpretation, and problem-solving: Apply critical thinking skills to analyze complex chemical problems and propose innovative solutions. Effective in interpreting experimental data using appropriate statistical methods and computational tools.

PSO 5. Effective communication: Communicate scientific ideas, research findings, and complex concepts effectively through written reports, research papers, and oral presentations.

PSO 6. Safety and ethical practices: Awareness of ethical principles and safety protocols in all aspects of chemical research and laboratory work.

PSO 7. Interdisciplinary knowledge and collaboration: Display the ability to integrate knowledge from various fields, collaborate with interdisciplinary teams, and apply chemical principles to solve problems in related areas, such as drug chemistry, environmental science, pharmaceuticals, biochemistry, material science, nanoscience, etc.

5. THE COURSE OUTCOMES

Course Outcomes (COs): Course outcomes are the objectives that are achieved at the end of any semester/year. For instance, if a student is studying a particular course, then, the outcomes would be concluded based on the marks or grades achieved in theory and practical lessons.

The COs are set at the beginning of the study of each course.

6. THE COURSE STRUCTURE, SCHEME & CREDITS

6.1 The course structure, syllabus, and scheme are given below.

Semester	Paper Code	Title	Hrs /wk	Exam Duration	Marks for ESA	Marks for CA	Total	Credit
I	MSCHD01C01	Theoretical Chemistry - I	4	3	60	15	75	4
	MSCHD01C02	Inorganic Chemistry - I	4	3	60	15	75	4
	MSCHD01C03	Organic Chemistry - I	4	3	60	15	75	4
	MSCHD01C04	Physical Chemistry - I	4	3	60	15	75	4
	MSCHD01C05	Inorganic Chemistry Practical - I	3	Carried over to semester - II				
	MSCHD01C06	Organic Chemistry Practical - I	3	Carried over to semester - II				
	MSCHD01C07	Physical Chemistry Practical - I	3	Carried over to semester - II				
		Total :	25		240	60	300	16
II	MSCHD02C08	Theoretical Chemistry - II	4	3	60	15	75	4
	MSCHD02C09	Inorganic Chemistry - II	4	3	60	15	75	4
	MSCHD02C10	Organic Chemistry - II	4	3	60	15	75	4
	MSCHD02C11	Physical Chemistry - II	4	3	60	15	75	4
	MSCHD01&02C05	Inorganic Chemistry Practical - I	3	6	40	10	50	2
	MSCHD01&02C06	Organic Chemistry Practical - I	3	6	40	10	50	2
	MSCHD01C&02C07	Physical Chemistry Practical - I	3	6	40	10	50	2
		Total :	25		360	90	450	22
III	MSCHD03001/02/03	Open Elective Paper I* (Multidisciplinary)	4	3	60	15	75	4
	MSCHD03C12	Inorganic Chemistry III	4	3	60	15	75	4
	MSCHD03C13	Organic Chemistry - III	4	3	60	15	75	4
	MSCHD03C14	Physical Chemistry - III	4	3	60	15	75	4
	MSCHD03C15	Inorganic Chemistry Practical - II	3	Carried over to semester - IV				
	MSCHD03C16	Organic Chemistry Practical - II	3	Carried over to semester - IV				
	MSCHD03C17	Physical Chemistry Practical - II	3	Carried over to semester - IV				
	MSCHD03C18	Industrial Visit/Institutional Visit/Internship		Carried over to semester - IV				
		Total :	25		240	60	300	16
IV	MSCHD04E01/02/03	Elective Paper II*	4	3	60	15	75	4
	MSCHD04E04/05/06	Elective Paper III*	4	3	60	15	75	4
	MSCHD03&04C15	Inorganic Chemistry Practical - II	3	6	40	10	50	2
	MSCHD03&04C16	Organic Chemistry Practical - II	3	6	40	10	50	2
	MSCHD03&04C17	Physical Chemistry Practical - II	3	6	40	10	50	2
	MSCHD03&04C18	Industrial Visit/Institutional Visit/Internship			20	5	25	2
	MSCHD04C19	Project (With Presentation)	8		60	15	75	6
	MSCHD04C20	Viva Voce (General)			40	10	50	4
		Total :	25		360	90	450	26

6.2 The semester-wise split-up of marks is given below.

Semesterwise Split-up of Marks

Sem	Hrs allotted	Marks for ESA	Marks for CA	Total Marks	Credit
I	25	240	60	300	16
II	25	360	90	450	22
III	25	240	60	300	16
IV	25	360	90	450	26
	100	1200	300	1500	80

6.3 Elective Papers: The M.Sc. Drug Chemistry students may choose one open elective (multidisciplinary) from the following set 1 for semester III, and two elective papers for semester IV from groups II and III.

ELECTIVE PAPERS		
Sem	Paper Code	Title
III	MSCHD03001	Food Chemistry
	MSCHD03002	Environmental Chemistry And Disaster Management
	MSCHD03003	Interdisciplinary topics and instrumentation techniques
IV	MSCHD04E01	Introduction To Drug Chemistry
	MSCHD04E02	Biochemistry And Biophysical Chemistry
	MSCHD04E03	Introduction To Computational Chemistry & Computational Drug Design
IV	MSCHD04E04	Advances in Drug Chemistry And Drug Design
	MSCHD04E05	Medicinal Chemistry
	MSCHD04E06	Advances in Drug Synthesis

6.4 Project Work and Viva Voce

a) Each student shall carry out project work in one of the broad areas of drug/ organic/ inorganic/theoretical/physical/ environmental chemistry (Preferentially Drug Chemistry) for a period of a minimum of 12 weeks duration in the IVth semester under the supervision of a teacher of the department. A student may, in certain cases be permitted to do

the project work in an industrial/research organization on the recommendation of the department coordinator. In such cases, one of the teachers from the department shall act as co-supervisor.

b) The candidate shall submit 2 copies of the dissertation based on the results of the project work at the end of the program.

c) Every student has to do the project work independently. No group projects are accepted. The project should be unique with respect to the title, project content, and project layout. No two project reports of any students should be identical, in any case as this may lead to the cancellation of the project report by the university.

d) The ESE of the project work shall be conducted by two external examiners. The evaluation of the project will be done in two stages.

i. Internal evaluation (supervising teacher/s will assess the project and award internal marks)

ii. External evaluation (by external examiners appointed by the university)

e) Pass conditions

i. The student shall declare to pass the project report course if she/he secures a minimum of 40% marks (internal and external put together). In an instance of the inability of obtaining a minimum of 40% marks, project work may be redone and the report may be resubmitted along with subsequent exams through the parent department. There shall be no improvement chance for the marks obtained in the project report.

f) Assessment of different components of the project may be taken as below

g) Viva voce shall be conducted by two examiners; both of them shall be external examiners. Viva voce is based on theory and practical papers of all semesters including elective papers

PROJECT

Internal (Viva) 20% of total		External (80% of Total)	
Components	**% of internal marks**	**Components**	**% of external marks**
Punctuality	10	Relevance of topic and Structure of Report	20
Use of data	10	Quality of Analysis/ use of statistical tools	20
Scheme Organization of	30	Findings and recommendations	20
Viva-voce	50	Presentation of Project Report	20
		Viva-voce	20

6.5 Internship/ Industrial Visit/ Institutional Visit

a) Internships provide hands-on experience in real-world chemistry settings, allowing postgraduates to apply their theoretical knowledge in practical scenarios. This experience enhances their understanding of laboratory techniques, equipment, and experimental procedures.

Each student shall undergo an internship for a period of a minimum of two weeks duration or visit a minimum of two or more institutions/ industries of national/international importance in any of the Ist to IVth semesters and the report should be submitted during IVth semester practical examination along with project evaluation / Viva voce.

b) The candidate shall submit a copy of the IV/internship report during the IVth semester project evaluation / Viva voce.

6.6 Continuous assessment

a) This assessment shall be based on a predetermined transparent system involving periodic written tests, assignments, and seminars in respect of theory courses and based on tests, lab skills, records, and viva in respect of practical courses.

b) The percentage of marks assigned to various components for internal is as follows

Theory		
No	**Components**	**% of internal marks**
1	Two test paper	50
2	Assignments	25
3	Seminars/Presentation of case study	25

Practicals		
No	**Components**	**% of internal marks**
1	Two test paper	40
2	Lab skill	20
3	Record	20
4	Viva	20

6.7 Grading system

The seven-point indirect grading system is followed and the guidelines for grading are as follows

GRADING PATTERN

Sl. No	% of Marks	Grade	Interpretation	Range of Grade Points	Class
1	90 and above	A+	Outstanding	9.0 - 10	First class with distinction
2	80 to below 9	A	Excellent	8.0 - 8.9	
3	70 to below 8	B	Very Good	7.0 - 7.9	First class
4	60 to below 7	C	Good	6.0 - 6.9	First class
5	50 to below 6	D	Satisfactory	5.0 - 5.9	Second Class
6	40 to below 5	E	Pass/Adequate	4.0 - 4.9	Pass
7	Below 40	F	Failed	0.0 - 3.9	Fail

6.8 Guidelines for the preparation of a dissertation on the project:

6.8.1. Arrangement of contents shall be as follows:

1. Cover page and title page
2. Bonafide certificate
3. Declaration by the student
4. Acknowledgement
5. Table of contents
6. List of tables
7. List of Figures
8. List of symbols, Abbreviations and Nomenclature
9. Chapters
10. Appendices
11. References

6.8.2. Page dimension and typing instructions:

The dimension of the dissertation on the project should be in A4 size. The dissertation should be typed on bond paper and bound using a flexible cover of thick white art paper or spiral binding. The general text shall be typed in the font style 'Times New Roman' and font size 12. For major headings font size may be 16 and minor heading 14. Paragraphs should be arranged in justified with a margin of 1.25 each on top. Portrait orientation shall be there on the left and right of the page. The content of the report shall be around 40 pages.

6.8.3. The Bonafide certificate shall be in the following format

CERTIFICATE

This is to certify that the project entitled .....(title) submitted to the Kannur University in partial fulfilment of the requirements of Post Graduate Degree in .....(subject), is a Bonafide record of studies and work carried out by ..... (Name of the student) under my supervision and guidance.

Office seal Signature, name, designation, and official address of the Supervisor.
Date

6.8.4. Declaration by the student shall be in the following format:

DECLARATION

I.....(Name of the candidate) hereby declare that this project titled .....(title) is a bonafide record of studies and work carried out by me under the supervision of ..... (Name, designation, and official address of the supervisor), and that no part of this project, except the materials gathered from scholarly writings, has been presented earlier for the award of any degree or diploma, or other similar title or recognition.

Date: Signature and name of the student

7. PATTERN OF QUESTION PAPERS

The pattern of question papers, time, and difficulty level for theory papers will be as follows

Section	Criteria	Time	Marks		Percentage	Revised Taxonomy/Level
A	5 out of 6 questions (short answer questions)	5 x 8 min = 40 min	5 × 3 =	15	25	1,2 (Remember, Understand)
B	3 out of 5 questions (paragraph questions)	3 x 20 min = 60 min	3 × 6 =	18	30	5, 6 (Evaluate, Create)
C	3 out of 5 questions (essay-type questions)	3 x 25 min = 75 min	3 × 9 =	27	45	3, 4 (Apply, Analyze)
			Total =	**60**	100	100

The distribution of questions will be as follows

Distribution of Questions				
Units	Unit 1	Unit 2	Unit 3	Unit 4
Number of Questions	4	4	4	4

SEMESTER-I		
MSCHD01C01: THEORETICAL CHEMISTRY - I		
Credit: 4		**TIME: 72 HOURS**

Course Outcomes: After the completion of the course, the learners should be able to

CO 1. Understand and examine the basic principles of Quantum Mechanics
CO 2. Apply the postulates of quantum mechanics to simple systems
CO 3. Make use of the approximation methods to calculate the properties of simple systems
CO 4. Demonstrate the principles of chemical bonding in diatomic and polyatomic molecules
CO 5. Apply HMO theory to simple conjugated systems

Course Content

UNIT -I	QUANTUM MECHANICS-I	18 Hours

Historical development of Quantum Mechanics- Max Plank's Quantum Theory of Radiation - Photoelectric effect- Black body radiation – Compton effect – Wave-particle duality of matter-de-Broglie concept – Electron diffraction – Davison and Germer Experiment – Electron double slit experiment- Stern- Gerlach Experiment- Heisenberg's uncertainty Principle. Complex Numbers – definition - complex conjugate absolute values of a complex number – complex functions. Schrödinger wave mechanics – Deduction of Schrodinger equation from classical wave equation. The physical meaning of wave function. Normalized and orthogonal function. Elements of operator algebra: definition – linear non–linear operators – commuting and non-commuting operators-vector operators – Laplacian operators and their expressions in spherical polar coordinates (derivation not required). Eigenfunctions and Eigenvalues– Hermitian operators. Formulation of quantum mechanics: The postulates of quantum mechanics – state function postulate – operator postulate – Eigen value postulate – Expectation value postulate – Postulate of time-dependent Schrödinger equation stationary states and time-independent Schrödinger equation.

UNIT – II	QUANTUM MECHANICS – II	18 Hours

Translational motion: Particle in a one-dimensional box-complete treatment – particle in a three-dimensional box (rectangular and cubical box) – degeneracy.

Quantum mechanics of vibrational motion One-dimension Harmonic oscillator – complete treatment – Hermite polynomials – Recursion formula- comparison of classical and quantum mechanical results.

Quantum Mechanics of rotational motion: Particle on a ring (Planar rigid rotator)- Particle on a sphere (Nonplanar rigid rotator) – the wave function in spherical polar co-ordinates – complete treatment – Legendre polynomial –Rodrigue's formula- spherical harmonies –

wave function in the real form- polar diagrams-

Quantum mechanics of Hydrogen like atoms: potential energy of hydrogen-like atoms – the wave equation in spherical polar co-ordinates – solution of the R, θ, ϕ equations – Laguerre polynomials – associated Laguerre polynomials – Discussion of the wave functions –radial function, radical distribution function and angular function and their plots– orbitals and orbital diagrams – their significance.

UNIT – III	QUANTUM MECHANICS – III	18Hours

Need of approximate methods in quantum chemistry: variation method – variation theorem with proof –illustration of variation theorem using a trial function [e.g., x (a-x)] for the particle in a 1D-box and using the trial function e -αr2 for the hydrogen atom, variation treatment for the ground state of helium atom;

Perturbation method: time-independent first-order correction to the energy and wave function, second-order correction to energy– illustration by application to particle in an ID-box with slanted bottom, perturbation treatment of the ground state of the helium atom. Electron spin and atomic structure: spin functions and operators –spin-orbit interactions – Angular momentum – commutation relations – operators Term symbols – Russel – Saunder's terms and coupling schemes – introduction to SCF methods – Hartree and Hartree – Fock's SCF.

UNIT – IV	CHEMICAL BONDING	18 Hours

Born – Oppenheimer approximation – essential principles of the MO method – MO treatment of Hydrogen molecule and the H_2+ ion – valence bond treatment of the ground state of hydrogen molecule – MO treatment of homonuclear diatomic molecules (quantitative) – Li_2, Be_2, N_2, O_2, O_2+, O_2-, F_2 and heteronuclear diatomic - LiH, CO, NO, HF – theory of chemical bonding for polyatomic molecules – *Ab initio* calculations – basic principles — basis sets – STO and GTO –Spectroscopic term symbols for diatomic molecules.

Localized bonds – hybridization and geometry of molecules – methane, ethene, acetylene (bond angle, dihedral angle, bond length, and bond energy) – HMO theory of ethylene, butadiene, and benzene - aromaticity- bond order, charge density, and free valence calculations

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3. A. K. Chandra, Introductory Quantum Chemistry – 4th Ed. Tata Mc Graw Hill
4. D. A. McQuarrie Quantum Chemistry, University Science Books
5. L. Pauling and W.B Wilson, Introduction to Quantum Mechanics, McGraw Hill
6. R. K. Prasad, Quantum Chemistry 4th Ed. New Age International
7. P. W. Atkins, Molecular Quantum Mechanics, Oxford University Press
8. M.S.Day and J.Selbin, Theoretical Inorganic Chemistry, East West Books
– Tamas Veszpremi and Miklos Feber, "Quantum Chemistry – Fundamentals to Applications" Springer.
9. Quinn – "Computational Quantum Chemistry – An Interactive Guide to Basis Set theory"- Ane Books Pvt. Ltd.
10. Thomas Engel- Quantum Chemistry and Spectroscopy, 4th Edition, Pearson

MSCHD01C02: INORGANIC CHEMISTRY - I

Credit: 4		**TIME: 72 Hours**

Course Outcomes: After the completion of the course, the learners should be able to

CO 1: Apply the theory of precipitation phenomena in the determination of metal ions
CO 2: Impart advanced knowledge of the theory of complexometric titration

CO 3: Predict the stabilities of complexes based on the HSAB principle

CO 4: Understand different types of Non- aqueous solvents and their applications

CO 5: Develop and attain advanced knowledge of nuclear Chemistry and radiation Chemistry and their applications

CO 6: Demonstrate the preparation, structure, and properties of compounds of Boron, Phosphorous, and Nitrogen

Course Content

UNIT – I	**THEORETICAL BASIS OF ANALYSIS**	**18 Hours**

Precipitation phenomena – precipitation from homogenous solution, organic precipitants in inorganic analysis (Dimethyl glyoxime, cupferron, oxine reagent, cupron, nitron, anthranilic acid) – extraction of metal ions – nature of extractants – distribution law – partition coefficients – types of extraction and applications

Analytical applications of complex formation; Gravimetric analysis - Ni, Cu, - Chelometric titrations (a detailed study) – titration curves with EDTA – feasibility of EDTA titration –

indicators for EDTA titration and its theory (a detailed study) – selective masking and demasking techniques – industrial application of masking

Automated Techniques – Flow injection Analysis – Method and Instrumentation

Electrogravimetry – Theory, apparatus, and application- Determination of copper.

UNIT–II	ACIDS, BASES, AND NON-AQUEOUS SOLVENTS	18 Hours

A generalized acid-base concept - Measure of acid-base strengths – gas phase basicities – proton affinities – gas phase acidities – proton loss gas phase acidities – electron affinities – systematic of Lewis acid-base interaction – bond energies – steric effect – proton sponges. Solvation effects and acid-base anomalies. Hard and soft acids and bases – classification – strength and hardness and softness – symbiosis – theoretical basis of hardness and softness – electron negativity and hardness and softness.

Superacids and bases – Types, examples, and applications

Classification of solvents – properties of nonaqueous solvents like HF, N_2O_4, and SO_2 – chemistry of molten salts as nonaqueous solvent systems – solvent properties – room temperature molten salts – nonreactivity of molten salts - solution of metals –

Ionic liquids as green solvents, room temperature ionic liquids, and supercritical fluids. Use of non-aqueous solvents in synthesis

UNIT – III	NUCLEAR AND RADIATION CHEMISTRY	18 Hours

Nuclear models – shell, liquid drop, Fermi gas, Collective and optical models – Assumptions, merits, and demerits– equation of radioactive decay – half-life and average life. Radioactive equilibrium – transient and secular equilibrium – Bethe's notation for nuclear processes - types of nuclear reaction –neutron capture cross section and critical size – principles and working of GM and scintillation counters.

Basic principles of nuclear reactors – types of reactors – PHWR, BWR

Elements of radiation chemistry – introduction- the interaction of ionizing radiation with matter. LET for charged particle due to collision with electron. Bremsstrahlung interaction of electromagnetic radiation with matter. Radiolysis of water - Radiation dosimetry - Fricke Dosimeter- Applications of radiation chemistry – Rock dating, Nuclear Activation Analysis, Tracer techniques, Medicine, Industry

UNIT–IV	BORON, PHOSPHORUS, AND NITROGEN COMPOUNDS	18 Hours

The neutral boron hydrides – structure and bonding topological approach to boron hydride structure – Styx number – synthesis and reactivity of neutral boron hydrides. Importance of

icosahedral framework of boron atoms in boron chemistry – closo, nido, and arachno structure – Wades rule – mno rules

Carboranes– Structure and classification - preparation and properties of dicarba-closododecaboranes ($C_2B_{10}H_{12}$ - ortho, meta, and para) - metallocarboranes – preparation and structure of metallo carboranes of Fe & Co

Phosphorous sulphides – P_4S_3, P_4S_5, P_4S_7, and P_4S_{10} – preparation, properties, structure, and uses. The phosphazenes (phosphonitrilic halides)

Sulphur nitrogen compounds – S_2N_2 and S_4N_4 – Polythiazyl, other S_XN_Y compounds. Their preparation properties, and structure.

Poly acids - Iso poly and heteropoly acids of Mo & W elements – Structure and formation

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4. G N Jeffery, J Basette, J Mendham and R C Denny, Vogel's textbook of quantitative chemical analysis (Vth edition), John Wiley and Sons
5. H Sisler, Chemistry of non-aqueous solvents, Reinhold
6. J E Huhee, Inorganic Chemistry Principles of Structure and Reactivity, Person Education India
7. G Friedlander and J W Kennedy, Introduction to radiochemistry, John Wiley and Son Inc
8. S Glasston, a Sourcebook on atomic energy, Van Nostrand
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11. S K Agarwal and Keemti Lal, Advanced Inorganic Chemistry, Pragati Prakashan 9th Edition 2009
12. B K Sharma, Instrumental Methods of Chemical Analysis, Goel Publishing House, 2000
13. Duward F Shriver, Peter William, Atkins, Cooper Harold Langford, Inorganic Chemistry
14. M G Arora and M Singh, Nuclear chemistry
15. Walter D Loveland, David J Morrissey, Glenn T Seaborg, Modern Nuclear Chemistry

16. Catherine E Housecroft and Alan G Sharpe. Inorganic Chemistry, 4th Edition, Pearson

17. George A Olah, G K Surya Prakash Superacid Chemistry, 2nd Edition, Wiley

MSCHD01C03: ORGANIC CHEMISTRY - I

Credit: 4		**TIME: 72 Hours**

Course Outcomes: After the completion of the course, the learners should be able to

CO 1. Study the various reaction intermediates in organic reactions.

CO 2. Investigate the role of reaction conditions and reagents in the generation of intermediates.

CO 3. Formulate a mechanism for the suggested reactions.

CO 4. Analyze the structure-property relations in aliphatic substitution reactions. Apply the concept of elimination to various organic molecules.

CO 5. Understand the various aromatic systems and their reactions. Classify molecules based on the aromatic behavior.

CO 6. Study the different photochemical reactions and apply them to natural photochemical reactions.

Course Content

UNIT- I	**REACTION INTERMEDIATES AND REARRANGEMENTS**	**18 Hours**

Structure, formation, and properties of carbenes, nitrenes, and arynes – singlet and triplet carbenes, nitrenes and arynes, Carbon free radicals: structure, formation, and stability. Structure, stability, and formation of Ylides, Enamines, 1,3-dithiane, Benzynes, and Enolates.

Molecular rearrangement mechanism. Carbon to carbon migration: Wagner Meerwein, Pinacol, Wolff, Benzilic acid, Demjanove, Dienone-phenol, Hoffmann-Martius. Carbon to nitrogen migration: Hofmann, Curtius, Schmidt, Lossen, Beckmann. Migration to electron-rich carbon: Wittig, Wittig-Hormer, Favorski, Stevens, Neber Orton, Bamberger. Migration to electron-deficient oxygen: Baeyer, villager, Darkin reaction. Aromatic rearrangements: benzidine, Fries, Von-Richter Sommlet-Hauser.

UNIT- II	SUBSTITUTION AND ELIMINATION REACTIONS	18 Hours

Aliphatic nucleophilic substitution reactions – saturated and unsaturated systems – Mechanism of nucleophilic substitution – SN2, SN1, SNi, SET. Neighbouring group participation – non-classical carbocations. Substitution at allylic and vinylic carbon atoms. Effect of substrate structure, attacking nucleophile, leaving group, and reaction medium on reactivity and regioselectivity. Aliphatic Electrophilic substitutions: SE1 SE2 and SEi mechanisms with suitable examples.

Elimination Reaction: Mechanistic and stereochemical aspects of E1, E2, and E1cB eliminations. The effect of substrate structure, base, leaving group, and reaction medium on elimination reactions. Elimination reaction in 4-t-Butylcyclohexyl tosylate (cis and trans), 2-Phenylcyclohexanol (cis and trans), Menthyl and neomenthyl chlorides, and benzene hexachlorides. Saytzev vs. Hofmann elimination, Bredt's rule, α- elimination, pyrolytic syn elimination (Ei) – Chugaev reaction, and Cope elimination. Dehydration of alcohols, Dehalogenation of vicinal dihalides, and Peterson elimination.

UNIT- III	AROMATICITY AND AROMATIC REACTIONS	18 Hours

MO description of aromaticity and antiaromaticity. Homoaromaticity. Aromaticity of annulenes and heteroannulenes, fused ring systems, fulvenes, fulvalenes, azulenes, pentalenes, and heptalenes. mesoionic compounds, metallocenes, cyclic carbocations, and carbanions. Effect of delocalized electrons on pKa.

Aromatic Electrophilic Substitution: Arenium ion mechanism, substituent effect on reactivity in mono and disubstituted benzene rings, *ortho/para* ratio, *Ipso* substitution. Relationship between reactivity and selectivity.

Aromatic Nucleophilic substitution: Addition-elimination (SNAr) mechanism, elimination-addition (benzyne) mechanism, *cine* substitution, SN1 and SRN1 mechanism. The effect of substrate structure, nucleophile, and leaving group on aromatic nucleophilic substitution. Nucleophilic Substitution of Pyridine-Chichibabin Reaction.

UNIT- IV	PHOTOCHEMISTRY	18 Hours

Photochemical excitation of molecules, spin multiplicity, Jablonski diagram, photosensitization, and quenching. Photochemistry of carbonyl compounds: Norrish type- I cleavage of acyclic, cyclic, and β, γ- unsaturated carbonyl compounds. Norrish type- II cleavage, photo reduction, photoenolization. Photocyclo- addition of ketones with unsaturated compounds: Paterno- Büchi reaction, photodimerization of α, β- unsaturated ketones, Photo rearrangements: Photo –Fries, di-π- methane, oxa di- π- methane, aza di- π- methane, lumi ketone rearrangements. Barton and

Hoffmann- Loeffler- Freytag reactions. Photo isomerization and dimerization of alkenes, photo isomerization of benzene and substituted benzenes, and photo-oxidation. Photochemistry of vision and photosynthesis.

REFERENCES:

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9. I L Finar, Organic Chemistry Volume 2, Pearson Education.
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11. Modern methods of organic synthesis, Carruthers,
12. P.S.Kalsi, Organic reactions & their mechanisms, 3/e revised, New Age International Publishers.
13. J. Sing and J. Sing, *Photochemistry and Pericyclic Reactions*, 3/e, New Age International, 2012.

MSCHD01C04: PHYSICAL CHEMISTRY - I

Credit: 4		**TIME: 72 Hours**

Course Outcomes: After the completion of the course, the learners should be able to

CO 1. Illustrate the concepts of the third law of thermodynamics and thermodynamic irreversibility.

CO 2. Analyze phase transitions and phase diagrams of three component systems.

CO 3. Develop an understanding of the theoretical aspects of electrochemical activities and various facets of electrochemistry.

CO 4. Interpret the mechanism of electrode-electrolyte interaction.

CO 5. Analyze different aspects of the electrode process.

CO 6. Illustrate the importance and concepts of electrochemistry in other fields like supercapacitors, batteries, and corrosion.

Course Content

UNIT-I	**THERMODYNAMICS AND PHASE EQUILIBRIA**	**18 Hours**

Thermodynamics: Third law of thermodynamics- need for third law, Nernst heat theorem, determination of absolute entropies using third law, Residual entropy. entropy changes in chemical reactions. Thermodynamic equations of state.

Partial molar quantities - chemical potential-variation of chemical potential with T&P- determination of partial molar volume and enthalpy. Thermodynamic functions of ideal gases, real gases, and gas mixtures- Entropy and free energy of mixing. Excess thermodynamic functions. Thermodynamics of irreversible processes with simple examples. The general theory of nonequilibrium processes. Entropy production. The phenomenological relations. Principle of microscopic reversibility, Onsager reciprocal relations. Application to the theory of diffusion, thermo-osmosis, and Thermoelectricity (Seebeck effect, Peltier effect, and Thomson effect).

Phase equilibria: Phase rule -Physical equilibria involving phase transition-criteria for equilibrium between phase-Three component system- graphical representations-solid liquid equilibria Ternary solution with common ion-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-II	**ELECTROCHEMISTRY**	**18 Hours**

The nature of electrolytes– Ionic mobilities- ion activity- ion-ion and ion -solvent interaction. Equilibrium properties of electrolyte solutions. Electrolytes of the first and second kind, - Influence of pressure and temperature on ion conductance-Walden's equation- Abnormal ion conductance-Derivation of Debye-Huckel Onsager equation- the validity of Debye-Huckel-Onsager equation for aqueous and non-aqueous solution-Deviation from Onsager equation-Conductance ratio and Onsager equation-Dispersion of conductance at high frequencies-Triple ion conductance minima-Equilibria in electrolytes-Association constant Ion-association-dissociation constant--- Activities and activity coefficient in electrolytic solutions.-Debye-Huckel limiting law and its various form, qualitative and quantitative tests of Debye-Huckel limiting equation. Osmotic coefficient- solubility product principle-solubility in the presence of common ion-activity coefficient and solubility measurement.

UNIT-III	**ELECTRODICS**	**18 Hours**

Liquid junction potential. The electrode double layer-electrode-electrolyte interface-Theory of

multilayer capacity. Electric capillary Lippmann -potential, Membrane-potential. Butler Volmer equation for simple electron transfer reaction-Transfer coefficient- Exchange current density Rate constants- Tafel equation and its significance.

Electrolytic polarization- dissolution and deposition potentials, concentration polarization. Decomposition voltage and its determination.

Overvoltage - hydrogen and oxygen overvoltage, metal deposition over-voltage, and their determination. Theories of overvoltage.

Cyclic Voltammetry- Theory and experimental setup, Cyclic voltammogram.

Polarography- Principle and instrumentation Dropping mercury electrode- half-wave potential and Ilkovic equation.

UNIT-IV	**APPLIED ELECTROCHEMISTRY AND CORROSION**	**18 Hours**

Energy storage devices: Batteries- Working of Lithium-ion battery. Basics of supercapacitors, Classification with examples. Electrostatic double layer capacitors (EDLC) and Psuedo capacitors- working and principle.

Corrosion: Thermodynamics of corrosion and electrode potentials. EMF of a cell-measurement- emf calculation of half cell potential-Nernst equation. Basis of Pourbaix diagrams- Diagrams of water, Fe, and Al. Limitations of Pourbaix diagrams. Kinetics of corrosion- Polarization and corrosion rate. Measurement of corrosion rate. Measurement of polarization- causes of polarization. Calculation of IR drops in an electrolyte. Influence of polarization on corrosion rate. Polarization diagram of corroding metals. Calculation of corrosion rate from polarization data. Theory of cathode protection. Passivity.

REFERENCES

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14. Fontana and Greene Corrosion Engineering:

15. What are batteries, fuel cells, and supercapacitors? *Chem Rev.2004,104,4245-4269*

16. Electrochemical methods: Fundamentals and application by Allen J. Bard and Larry R Faulkner.

17. Lithium-ion batteries basics and applications by Reiner Korthaneur.

18. Electrochemical supercapacitors: Scientific fundamentals and Technological applications, B.E. Conway.

SEMESTER – II

MSCHD02C08: THEORETICAL CHEMISTRY - II

Credit: 4		**TIME: 72 Hours**

Course Outcomes: After the completion of the course, the learners should be able to

CO 1. Analyze the symmetry aspects of a given molecule and find its point group

CO 2. Explain the basic principles of group theory and construction of the character table

CO 3. Apply the principles of group theory to spectroscopy and chemical bonding

CO 4. Understand the interaction of matter with radiation in terms of the relation with the molecular energy levels.

CO 5. Explain and apply the selection rules pertaining to various molecular spectral transitions.

CO 6. Develop advanced awareness about the various spectroscopic techniques- IR, Raman, Electronic, and NMR

Course Content

UNIT – I	**MOLECULAR SYMMETRY, GROUPS, MATRICES**	**18 Hours**

Symmetry elements and symmetry operations in molecules –point groups and their symbols – Classification of point groups– Systematic identification of point groups- order of a group- finite, Infinite, abelian, non-abelian, cyclic, and non-cyclic groups – sub-groups- Mathematical groups and its properties- group multiplication tables of C_{2v}, $C_{2h,}$ and C_{3v} –Rearrangement theorem- classes in a group and similarity transformation – Matrices – addition and multiplication of matrices – the inverse of a matrix- the character of a matrix- block diagonalization – matrix notation of symmetry operations –General expression for the character of an operation-

representation of groups – construction of representation using vectors and atomic orbital as the basis – Γcart, Representation generated by Cartesian coordinates positioned on the atoms of a molecule (H_2O and SO_2 as examples) -Γregular – reducible and irreducible representations – construction of irreducible representation by reduction.

UNIT II	THEORY OF MOLECULAR SYMMETRY AND APPLICATIONS OF GROUP THEORY	18 Hours

Great Orthogonality Theorem (GOT) (without proof) – Rules derived from GOT- construction of irreducible representation using GOT – construction of character tables (C_2v, C_2h, C_3v, C_4v). Four areas of Character Table- Mulliken symbols- Reduction formula.

Applications of Group theory- Applications to chemical bonding – construction of hybrid orbitals – BF_3 CH_4, PCI_5 as examples- Application to MO theory-. Group orbitals and their construction-Projection Operator method and pictorial method- Transition Moment Integral. Examples H_2O, NH_3, and octahedral complexes (sigma bonding using the pictorial method)

Applications in IR and Raman spectroscopy: symmetry aspects of molecular vibrations – Normal mode Analysis - selection rules for IR and Raman –-complementary character of 1R and Raman spectra – determination of the active 1R and Raman vibrational modes of H_2O, NH_3, CH_4, BF_3, N_2F_2

UNIT – III	SPECTROSCOPY	18 Hours

General theory: electromagnetic radiation, regions of the spectrum, the interaction of electromagnetic radiation with matter and its effect on the energy of molecules – Natural line width and broadening. The intensity of spectral lines – Einstein Coefficient- Rotational, vibrational, and electronic energy levels, and selection rules – transition moment integral

Microwave spectroscopy: Classification of molecules – rotational spectra of diatomic and polyatomic molecules – Rigid and non-rigid rotator models – Determination of bond lengths – isotope effect on rotation spectra – applications.

Vibrational and vibration – rotation spectra: Vibrational energies of diatomic molecules – the interaction of radiation with vibrating molecules – anharmonicity of molecular vibrations, fundamental, overtones and hot bands – Degree of freedom of polyatomic molecules and nature of molecular, vibrations (e.g.. CO_2 and H_2O). vibration – rotation spectra of diatomic and polyatomic molecules selection rules – determination of force constant.

Raman Spectroscopy: Theory of Raman spectra (classical and quantum mechanical theory) –

pure rotational vibrational Raman spectra, vibrational –rotational Raman spectra, selection rules – mutual exclusion principle – Applications of Raman and I R spectroscopy in the elucidation of molecular structure (eg. H_2O, N_2O and CO_2 molecules)

UNIT –IV	**SPECTROSCOPY II**	**18 Hours**

Electronic spectra: Electronic spectra of diatomic molecules – vibrational coarse structure and rotational fine structure of electronic spectrum – Franck – Condon principle – Types of electronic transitions – Fortrat diagram – Dissociation and pre – dissociation – calculation of heat of dissociation.

Nuclear Magnetic Resonance Spectroscopy: General theory – magnetic properties of nuclei – theory and measurement techniques – population of energy levels – solvents used –chemical shift and its measurement – factors affecting chemical shift – Nuclear resonance – Relaxation methods – integration of NMR signals – spin sin coupling – coupling constant j and factors affecting it – shielding and de shielding – chemical shift assignment of major functional groups – classification (AX, AB, ABX,) spin decoupling – Application to the study of simple molecules.

REFERENCES

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2. L H Hall "*Group Theory and Symmetry in Chemistry",* McGraw Hill.
3. V Ramakrishnan and M S Gopinathan, *"Group Theory in Chemistry"* Vishal Publications, 1992.
4. Banwell and Mc Cash "*Fundamentals of Molecular Spectroscopy",* Tata McGraw Hill
5. G Aruldas *"Molecular Structure and Spectroscopy",* Prentice Hall,
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10. Thomas Engel "*Quantum Chemistry and Spectroscopy"* – Pearson.
11. Quinn "*Computational Quantum Chemistry – II: The Group Theory Calculator"* – Ane Books
12. H.Kaur "Spectroscopy" 3rd Edition Pragati Prakashan Meerut

MSCHD02C09: INORGANIC CHEMISTRY - II

Credit: 4		TIME: 72 Hours

Course Outcomes: After the completion of the course, the learners should be able to

CO 1: Develop advanced knowledge about the VB and MO theory of coordination compounds

CO 2: Explain the spectroscopic features of complexes and interpret the spectra of complexes

CO 3: Describe the magnetic behaviour of complexes and apply magnetic properties in the structural determination of complexes

CO 4: Understand the various mechanisms operative in inorganic complexes during substitution and in electron transfer reactions.

CO 5: Explain different physical methods in Inorganic chemical analysis

Course Content

UNIT – I	COORDINATION CHEMISTRY – I	18 Hours

Coordination numbers 2 to 12 and geometry – VB theory, assumption, and limitations. Crystal field theory of coordination compounds – d-orbital splitting in octahedral, tetrahedral, and square planar fields. Crystal field effect on ionic radii and lattice energies – Jahn Teller effect – evidence for ligand field splitting – spectrochemical series. MOT in coordination compounds – MO energy level diagrams for octahedral, tetrahedral, and square planar configuration with and without π bonding. Effect of π bonding in stability – nephelauxetic series – experimental evidence for metal-ligand. Covalent bonding in the complex. Comparison of three theories as applied to metal complexes.

UNIT – II	COORDINATION CHEMISTRY – II	18 Hours

Spectroscopic ground states – term symbols for d^n ion. selection rules for d-d transitions – effect of spin-orbit coupling and vibronic coupling on electronic transitions - Orgel diagram of transition metal complexes(d^1 to d^9 configurations) Tanabe Sugano diagrams - Charge Transfer Spectra Magnetic behaviors – susceptibility, measurements – Gouy method diamagnetic corrections. Spin-only value – orbital contributions – spin-orbit coupling, ferro, and antiferro magnetic coupling – spin cross-over system – Temperature dependence of magnetic behaviour - Applications of magnetic measurements to structural determinations of transition metal complexes.

UNIT – III	COORDINATION CHEMISTRY III	18 Hours

The reaction of metal complexes: Stability constants – chelate effect – Irwing-Willian order of stability. Factors affecting the stability of metal complexes. Determination of binary formation constants by pH meter and spectrophotometry – Job's Method - energy profile of a reaction

Reaction of complexes: Ligand substitution reactions (Square planar and octahedral complexes). Rates of ligand substitutions, classification of mechanisms. The nucleophilicity of the entering group, The shape of the transition states, The activation of octahedral complexes, Base hydrolysis, stereochemistry, and Isomerisation reactions. A brief study of redox reaction – Outer sphere and Inner sphere mechanism – Marcus -Husch Theory

UNIT– IV	**PHYSICAL TECHNIQUES IN INORGANIC CHEMISTRY**	**18 Hours**

Study of inorganic compounds by the following methods - Diffraction methods – X-ray diffraction, neutron diffraction

UV, IR, Raman Spectroscopic Methods, Resonance technique – nuclear magnetic resonance, electron paramagnetic resonance, Mossbauer spectroscopy

Ionization-based techniques – photon electron spectroscopy, x-ray absorption spectroscopy, mass spectrometry

Chemical analysis – atomic absorption spectroscopy, CHN Analysis, X-ray fluorescence elemental analysis

Magnetometry – electrochemical techniques

REFERENCES

1. S F A Kettle, Coordination Chemistry, Thomas Nelson and Sons
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6. R Gopala and V N Ramalingam, Concise Coordination Chemistry, Vikas Publishing House Pvt Ltd
7. M C Day and J Selbin, Theoretical Inorganic Chemistry, Affiliated EAST West Press
8. J E Huheey, Inorganic chemistry principles of structure and reactivity, Pearson Education India
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MSCHD02C10: ORGANIC CHEMISTRY - II

Credit: 4		TIME: 72 Hours

Course Outcomes: After the completion of the course, the learners should be able to

CO 1. Understand the basic concepts of conformational analysis and evaluate the effect of conformational changes in molecular reactions.

CO 2. Apply the basic concepts of stereochemistry in stereoselective asymmetric synthesis.

CO 3. Understand molecular orbital approaches in pericyclic reactions.

CO 4. Formulate mechanisms for pericyclic reactions and problems.

CO 5. Understand and analyze various name reactions in organic chemistry.

CO 6. Generate mechanisms for reactions and understand the basic concepts for asymmetric synthetic reagents.

Course Content

UNIT – I	CONFORMATIONAL ANALYSIS	18 Hours

Difference between configuration and conformation. Internal factors affecting the stability of molecules – dipole interaction, bond opposition strain, bond angle strain. Conformational analysis of cyclic compounds: Cyclohexane Interconversion of axial and equatorial bonds in chair conformation of cyclohexane–the distance between the various H atoms and C atoms in chair and boat conformations.

Monosubstituted cyclohexane–methyl and t-butyl cyclohexanes–flexible and rigid systems. Conformation of substituted cyclohexanone, 2-bromocyclohexanone, dibromocyclo hexanone, (cis & trans), 2-bromo-4,4-dimethyl cyclohexanone. Anchoring group and conformationally biased molecules. Octant and axial and halo ketones rules. Stereochemistry of fused, bridged, and caged ring systems-decalins, norbornane, barrelene, and adamantanes.

UNIT – II	STEREOCHEMISTRY AND ASYMMETRIC SYNTHESIS	18 Hours

Molecules with C, N, S based chiral centers. Axial, planar, and helical chirality with examples of R and S nomenclature using Cahn-Ingold-Prelog rules. Optical purity, enantiomeric excess, and diastereomeric excess and their determination. Topicity and pro stereoisomerism, prochiral centre, enantiotopic, homotopic, diastereotopic hydrogen atoms.

Asymmetric synthesis, need for asymmetric synthesis, stereoselectivity, and stereospecificity. Strategies in Asymmetric Synthesis: Chiral pool: Amino acids in the synthesis of benzodiazepines-conversion of L-tyrosine into L-Dopa; synthesis of beetle pheromone component (S)- (–)-ipsenol from (S)-(–)-leucine, Carbohydrates – (R) Sulcatol from 2-deoxy-D-ribose. Cram's rule, Cram's

chelation control, Prelog's rule, and Felkin-Anh model.

UNIT III	PERICYCLIC REACTIONS	18 Hours

Symmetry properties of MOs – LCAO-MO theory of simple conjugated polyenes and cyclic polyenes – classification of pericyclic reactions- electrocyclic, cycloaddition, sigmatropic, chelotropic, and group transfer reactions. Mechanism and stereo course of electrocyclic, cyclo addition, and sigmatropic reactions.

Analysis of electrocyclic, cyclo addition, and Sigmatropic reactions by FMO, Woodward-Hoffmann Selection Rule, and Huckel-Mobius Method. Correlation diagram approach for electrocyclic, and cyclo addition reactions. Study of Electrocyclic Reactions: Nazarov cyclization. Study of Cycloaddition reactions: Stereo and Regiochemistry of Diels –Alder reaction, Intramolecular, Asymmetric, and retro Diels –Alder reaction. 1,3-dipolar cycloaddition, Ketene [2+2] cycloaddition. Sigmatropic reaction: [3,3] Cope rearrangement, Oxy-cope rearrangement, Aza cope rearrangement, classes, thia-claisen rearrangement, Fluxional molecules. [2,3] sigmatropic rearrangement, [5,5] sigmatropic rearrangement. Group transfer reactions: inter and intramolecular ene reactions, Carbonylene reaction, metallo-ene reaction. Chelotropic reactions: (2+2) chemotropic cycloaddition, (4+2) chelotropic cycloaddition, stereochemistry of chelotropic reactions

UNIT -IV	ORGANIC REACTIONS AND REAGENTS	18 Hours

Mannich, Simon-Smith, Heck, reactions. Michael, Prevost, and Woodward hydroxylation of alkenes, Shapiro reaction, Sharpless asymmetric epoxidation, ring formation by Dieckmann, Thorpe, and Acyloin condensation. Robinson ring annulations, reduction, and oxidation in synthesis – catalytic hydrogenation. Alkali metal reduction. Birch reduction. Wolff-Kishner reduction, Huang-Milon modification. Clemmenson reduction. LAH, DIBAL, sodium borohydride as reductance. Oppenauer oxidation. HIO_4, OsO_4, and mCPBA and their applications. Synthetic applications of the following reagents – Gillman's reagent, LDA, 1, 3 dithianes, DDQ, DDC, SeO_2, Bakers yeast, NBS, Wilkinsons's catalyst. Asymmetric reductions using BINAL-H. Asymmetric hydroboration using IPC2BH and IPCBH2. Reduction with CBH reagent.

REFERENCES

1. E.L. Eliel, S.H. Wilen, Stereochemistry of Organic Compounds, John Wiley & Sons,1994.

2. D. Nasipuri, Stereochemistry of Organic Compounds: Principles and Applications, 3/e, New Age Pub., 2010.

3. P. S. Kalsi, Stereochemistry, 4/e, New Age International Ltd.

4. P.S. Kalsi, Organic reactions & their mechanisms, 3/e revised, New Age International Ltd.

5. G. L. D. Krupadanam, Fundamentals of Asymmetric Synthesis, Universities Press, 2013.
6. S. Sankararaman, *Pericyclic Reactions-A Textbook: Reactions, Applications and Theory,* Wiley VCH, 2005.
7. I. Fleming, *Molecular Orbitals and Organic Chemical Reactions*, Wiley, 2009.
8. J. Sing and J. Sing, *Photochemistry and Pericyclic Reactions*, 3/e, New Age International, 2012.
9. I. Fleming, *Selected Organic Synthesis*, John Wiley and Sons, 1982.
10. T. Landbery, *Strategies, and Tactics in Organic Synthesis*, Academic Press, London,1989.
11. E. Corey and I.M. Chang, *Logic of Chemical Synthesis*, John Wiley, New York, 1989.
12. J. Clayden, N. Greeves, S. Warren, P. Wothers, Organic Chemistry, Oxford University Press, 2004.
13. R.O.C.Norman & J.M.Coxon, Principles of Organic Synthesis, 3/e, Nelson Thornes
14. J. March, M.B. Smith, March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 6/e, Wiley, 2007.
15. Modern methods of organic synthesis Carruthers,
16. H O House, Modern synthetic reactions
17. Fieser and Fieser, Reagent in organic synthesis

MSCHD02C11: PHYSICAL CHEMISTRY - II

Credit: 4		**TIME: 72 Hours**

Course Outcomes: After the completion of the course, the learners should be able to

CO 1. Apply the theory and methods of the statistical approach of thermodynamics.

CO 2. Analyze different classical and quantum mechanical distribution functions.

CO 3. Interpret classical and quantum statistical mechanics, including Boltzmann, Fermi-Dirac, and Bose-Einstein statistics.

CO 4. Illustrate band theory and the reciprocal lattice (k-space) formalism in terms of the crystal lattice.

CO 5. Analyze the theory of X-ray diffraction in solids.

CO 6. Develop an idea of different solid properties, focusing on electric and magnetic properties.

Course Content

UNIT-I	**STATISTICAL THERMODYNAMICS -I**	**18 Hours**

Distinguishable and Indistinguishable particles, phase space, Ensemble, Macrostates, and microstates. Stirlings approximation- Thermodynamic probability --Derivation of Maxwell-

Boltzmann distribution law - – Partition function- physical significance- total partition function; Separation of Molecular partition function - Translational, Rotational, vibrational, electronic and nuclear partition function. Rotational temperature- Fundamental vibrational temperature-Thermal de-Broglie wavelength. Heat capacity of gases- Classical and quantum theories-Equipartition principle - Heat capacity of Hydrogen – Ortho and Para-Hydrogen. The atomic crystals: Einstein's theory of atomic crystal - Debye's modification of Einstein's model.

UNIT-II	**STATISTICAL THERMODYNAMICS -II AND QUANTUM STATISTICS**	**18 Hours**

Partition function and thermodynamic functions- Partition function and equilibrium constants - Equation of state – Sackur Tetrode equation- Statistical formulation of the third law of thermodynamics.

Need for quantum statistics, Bose-Einstein statistics: Bosons-Bose Einstein distribution law, Bose-Einstein condensation, liquid helium, Fermi- Dirac statistics: Fermions- Fermi- Dirac distribution law, application to electrons in metals- Thermionic emission. Comparison of three statistics.

UNIT-III	**IMPERFECTIONS IN SOLIDS AND CRYSTALLOGRAPHY**	**18 Hours**

IMPERFECTIONS IN SOLIDS: Perfect and imperfect crystals, Classification; point defects, line and plane defects, vacancies- Thermodynamics and calculation of a number of defects of Schottky and Frenkel defects and formation of color centres, non-stoichiometric defects. Structures of FeO (Rock salt structure) and TiO_2(anatase and rutile structure only)

CRYSTALLOGRAPHY: Isomorphism and polymorphism- Miller indices- diffraction of X-rays- Laue equation- Bragg's Law - - Bragg Method-Debye-Scherrer method of X-ray structure analysis of crystals, indexing of reflections, identification of unit cells from systematic absence in diffraction pattern-structure of simple lattice - X-Ray intensities-structure factor and its relation to intensity and electron density-phase problem.

UNIT-IV	**PROPERTIES OF SOLIDS**	**18 Hours**

Electronic structure of solids-band theory and band structure of conductors, insulators, and semiconductors. Refinement to simple band theory - k-space and Brillouin Zones.

Electrical properties- electrical conductivity- Hall effect- dielectric properties- piezoelectricity- Ferroelectricity and conductivity.

Magnetic properties- diamagnetism- paramagnetism- Ferri, anti-ferro and ferromagnetism.

Superconductivity in metals - BCS theory- Meissner effect -type I & II superconductors.

Transition metal Oxides –Structure of Spinels, Inverse-spinels, and Perovskites, application of perovskites in solar cells.

Solid state lighting: Organic Light Emitting Diodes (OLEDs) - Principle, Device Architecture, Advantages and Disadvantages.

Quasicrystals -Basic introduction and applications only.

REFERENCES

1. M.C. Gupta-"Elements of Statistical Thermodynamics-New Age International.

2. L.K Nash-"Elements of Statistical Thermodynamics-Addision Wesley publishing.

3. Kistinand Sorfuran-"A course on statistical thermodynamics"-Academic 1971.

4. D.A.McQuarie-"Statistical thermodynamic"-HarperandRow1973.

5. D.K. Chakraharth-"Solid state chemistry"-New age publication.

6. I.V.Azaroof-"Introduction to solids"-McCrawHil.

7. Lesley E. Smart and Elaine A. Moore. "Solid state chemistry an introduction" Third edition, 2005. Taylor and Francis group.

8. A.R.West, Solid State Chemistry and its Applications, (1984) John Wiley and Sons, Singapore

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11. Molewyn Hughes-"Physical chemistry"-Pergamon press. 24. S. Glasstone and H.S. Taylor-"Treatise of Physical Chemistry"-Dvan Nostrand.

12, Feridoun Samavat*, Mohammad Hossein Tavakoli, Safdar Habibi, Babak Jaleh, Parisa Taravati Ahmad, Open Journal of Physical Chemistry, 2012, 2, 7-14

MSCHD01&02C05: INORGANIC CHEMISTRY PRACTICAL– I

(1st and 2nd semester)

Credit: 2		**TIME: 108 Hours**

Course Outcomes: After the completion of the course, the learners should be able to

CO 1: Identify advanced laboratory practices and develop laboratory skills through hands-on experiences.

CO 2: Identify the cations including rare elements, in a mixture of unknown salts

CO 3: Analyze metal ions using the volumetric method

CO 4: Analyze water quality parameters like hardness and DO

CO 5: Synthesize and characterize metal complexes of historical importance by various physicochemical methods

CO 6: Record, interpret, and analyze UV-Vis and IR spectra, TG curves, and XRD patterns of different metal complexes

CO 7: Predict the spectral characteristics of a given metal complex.

Course Content

Course Content:

Part 1: Separation and identification of four metal ions of which two are rare/ less familiar such as Tl, W, V, Se, Te, Ti, Ce, Th, Zr, U, Mo, and Li (interfering acid radicals not present). Confirmation by spot test. (Minimum 10 mixtures are to be recorded)

Part 2:

1) Volumetric estimation
   a) EDTA – Al, Ca, Cu, Ni, Co, Hardness of water
   b) Cerimetry – Fe(II), nitrate
   c) Estimation of Dissolved Oxygen by Winkler's method by titration
2) Preparation of the metal complexes, checking metal content and their characterization using UV-Vis spec / IR spec / TG & DTA /Magnetic susceptibility/ XRD data: Nickel (dimethyl glyoxime), Potassium trioxalatochromate (III), Tetraammoniumcopper (II) sulphate and Hexamminecobalt (III) chloride, and Potassiumhexathiocyanato chromate(III).

   [A minimum of 16 experiments to be recorded]

REFERENCES

1. A. I. Vogel, A Text Book of Qualitative Inorganic Analysis, Longman 5th edition, 1979.
2. G H Jeffrey, J Bassette, J Mendham and R C Denny, Vogel's textbook of quantitative inorganic analysis, Longman, 1999
3. J. Derek Woollins, Inorganic Experiments, 3rd ed, Wiley, 2010

4. G S Vehla, Vogel's quantitative inorganic analysis (7th edition), Longman 2001
5. D. A. Skoog and D. M. West, Analytical Chemistry: An Introduction, Saunders College Publishing, 4th edition, 1986.
6. W. G. Palmer, Experimental Inorganic Chemistry, Cambridge University,
7. V. Ramanujam, Inorganic Semimicro Qualitative analysis, 3rd edition, The National Publishing Company, Chennai 1974.

MSCHD01&02C06: ORGANIC CHEMISTRY PRACTICAL – I
(1st and 2nd SEMESTER)

Credit: 2		**Time: 108 Hours**

Course Outcomes: After the completion of the course, the learners should be able to

CO 1. Develop hands-on laboratory experience in the separation and purification of organic compounds.
CO 2. Analyze organic compounds and acquire lab skills in the synthesis of organic compounds.
CO 3. Determine physical constants and purification techniques
CO 4. Develop skills in chromatography
CO 5. Synthesize some simple organic medicinal compounds.

Course Content

Course Content

1) Analysis of organic binary mixtures (minimum 10 binary mixtures):

Separation of the binary mixture using physical and chemical methods. Checking its purity by Boiling points and Melting points. Preparation of the derivative of the compounds. The following types are expected:

(i) Solid-Solid (ii) Non-volatile liquid & Non-volatile liquid (iii) Water-soluble/insoluble solid and non-volatile liquid with compounds from the same or different chemical classes in all three categories.

2) One-stage Preparation of organic compounds (minimum 10 compounds):

Single-stage preparation involving nitration, halogenation, oxidation, reduction, alkylation, acylation, condensation, and rearrangements. Prepare medicinally important compounds and Heterocyclic compounds.

Purify the synthesized compound by means of recrystallization.

Spot TLC, report the R_f value, and check the completion of the reaction and purity of the compound.

3) Synthesis of the following organic medicinal compounds (minimum 2 compounds):

Paracetamol, Sulphanilamide, Aspirin, Sulphasalazine, Benzocaine, Phenytoin, Antipyrine (Exhibit during examinations)

[A minimum of 16 experiments to be recorded]

REFERENCES

1. A I Vogel, A textbook of practical organic chemistry, Longman
2. A I Vogel, Elementary practical organic chemistry, Longman
3. F G Mann and B C Saunders, practical organic chemistry, Longman
4. Shriner and Others, Systematic identification of organic compounds
5. Dey, Sitharaman and Govindachari, A laboratory manual of organic chemistry
6. PR Singh, DC Gupta & KS Bajpai, Experimental organic chemistry vol I & II
7. Vishnoi, Practical organic chemistry
8. Fieser, Experiments in Organic chemistry
9. Joseph Sharma, Gunter Zweig, TLC and LC Analysis of international importance, Vol. VI and VII, Academic Press
10. A. Kar, Advanced Practical Medicinal Chemistry, New Age International,2007
11. K A Connors, A Textbook of Pharmaceutical Analysis, John Wiley and sons, 2007
12. A O Bentley, J E Driver, Bentley and Divers Textbook of Pharmaceutical Chemistry, 7th Edn, Oxford University Press, 1960.

MSCHD01&02C07: PHYSICAL CHEMISTRY PRACTICAL – I

(Ist and 2nd SEMESTER)

Credit: 2		**Time: 108 Hours**

Course Outcomes: After the completion of the course, the learners should be able to

CO 1. Correlate and experimentally verify basic electrochemical principles related to conductance, mobility, and activities of ions

CO 2. Estimate concentration and molecular weights using cryoscopic methods

CO 3. Analyze physical constants like viscosity to determine the composition and molecular weights in the solution

CO 4. Perform electrochemical titrations in the laboratory by measuring the conductance and potential of solutions, and determination of dissociation constants of acids.

CO 5. Apply Physical chemistry concepts in the areas of phase equilibrium.

Course Content

1) Conductivity experiments

Equivalent conductance of weak acids – verification of Ostwald's dilution law –calculation of dissociation constant

Equivalent conductance of strong electrolytes (KCl). Verification of Onsagar equation

The activity coefficient of zinc in 0.002 M $ZnSO_4$ using the Debye-Huckel limiting law

Solubility product of sparingly soluble salts (AgCl-$BaSO_4$)

Conductance titrations. HCl vs NaOH, (HCl+ HOAc) vs NaOH, $AgNO_3$ vs KCl

2. Solubility and Heat of solution

Heat of solution from solubility data – analytical method and graphical method (ammonium oxalate and succinic acid)

3. Molecular weight determination

Molecular weight determination: Cryoscopic method and the transition temperature method. The molecular weight of a solid using a solid solvent by cooling curve method (solvents – naphthalene, biphenyl, diphenylamine, p-dichloro benzene). Molecular weight determination by the study of depression in transition temperature (sodium acetate, sodium thiosulphate, and strontium chloride)

4. Cryoscopic study

Study of $2KI + HgI_2 \rightarrow K_2HgI_4$ Reaction in water and determination of concentration of KI solution

5. Refractometry

Determination of molar refraction of pure liquids (water, methanol, ethanol, chloroform, carbon tetrachloride, glycerol). Determination of the composition of mixture (alcohol-water, glycerol-water, KCl-water)

6. Viscosity

Determination of viscosity of pure liquids (water, methanol, ethanol, glycerol, benzene, nitrobenzene, carbon tetrachloride). Composition of the binary liquid mixture (benzene-nitrophenol, water-alcohol). Determination of molecular weight of a polymer (polystyrene in toluene)

7. Potentiometry

The electrode potential of Zn and Ag electrodes in 0.1 M and 0.001 M solutions at 25 °C and determination of standard potentials. The mean activity coefficient of an electrolyte at different molalities by EMF method. Dissociation of the strength of the given HCl solution by the different potentiometric titration. Dissociation constant of acetic acid in DMSO, DMF, acetone, and dioxin by titrating with sodium hydroxide. Potentiometric titration. Acid-base titration, redox titration, and the

mixture of HCl and HOAc.

8. Phase rule

a) Solid and liquid equilibria: construction of phase diagram of simple eutectics, systems with congruent melting points, and solid solutions. Determination of the composition of unknown mixtures. Analytical and synthetic methods for the determination of solubilities and heat of solution

b) Partially miscible liquids: critical solution temperature, the influence of impurities on the miscibility temperature (KCl, NaCl, and /or succinic acid). Determination of the composition of unknown mixtures.

c) Completely miscible systems: construction of phase diagram of a two-component liquid system. Zeotropic and azeotropic

d) Three-component systems: with one pair of partially miscible liquids. Construction of phase diagrams of tie lines. Compositions of homogenous mixtures.

(A minimum of 20 experiments to be recorded covering all units)

REFERENCES

1. A Findlay and J A Kitchener, Practical physical chemistry, Longman
2. F Daniels and J H Mathews, Experimental physical chemistry, Longman
3. A M James, Practical physical chemistry, J A Churchill
4. H H Williard, L L Merritt and J A Dean, Instrumental methods of analysis, Affiliated East West press
5. D P Shoemaker and C W Garland, Experimental physical chemistry, McGraw Hill
6. W G Palmer, Experimental physical chemistry, Cambridge University Press

(A minimum of 20 experiments to be recorded covering all units)

SEMESTER III
MSCHD03C12 INORGANIC CHEMISTRY III

Credit: 4		**Time: 72 Hours**

Course Outcomes: After the completion of the course, the learners should be able to

CO 1 : To gain advanced knowledge about the transition metal carbonyls
CO 2 : To explain the metallurgical operations of rare earths from their ores
CO 3: To discuss the chemical and physical properties of Lanthanides and Actinides
CO 4: To discuss the general methods of preparation and properties of organometallics of main group elements
CO 5: To explain the different types of reactions shown by organometallic compounds

CO 6 : To study the applications of organometallic compounds in catalysis
CO 7: To distinguish essential and non-essential elements and to explain their significance in biological systems and medicines

Course Content

UNIT – I	**TRANSITION METAL CARBONYLS AND RELATED COMPOUNDS**	**18 Hours**

Introduction – preparation and properties of transition metal carbonyls – structures of transition metal carbonyl, structures of some carbonyls like $Ni(CO)_4$, $Fe(CO)_5$, $Cr(CO)_6$, $Fe_2(CO)_9$, $Co_2(CO)_8$, $Mn_2(CO)_{10}$, $Tc_2(CO)_{10}$, $Re_2(CO)_{10}$, Metal-metal bonding – Rhenium complexes , Carbonyl clusters (low nuclearity carbonyl clusters (LNCC) – Os_3CO_{12}, Ir_4CO_{12} and high nuclearity carbonyl clusters (HNCC) – Rh_6CO_{16}, and Mingo's Rule (polyhedral skeletal electron pair approach) – carbonyl hydrides and carbonylate anions and cations – carbonyl halides – phosphene and phosphorous trihalides complexes. Dinitrogen complexes – nitric oxide complexes – cyano complexes

UNIT – II	**METALLURGY AND CHEMISTRY OF f BLOCK ELEMENTS**	**18 Hours**

Thermodynamic aspects of extraction. Ellingham diagrams – Lattimer and Frost diagrams. Extraction, properties and uses of thorium, uranium, and plutonium. Beach sands of Kerala – important components and their separation from-monazite & ilmenite

Lanthanides:- electronic structure, oxidation states – chemical properties of +2,+3 and +4 oxidation state – lanthanide contraction – spectral and magnetic properties. Co-ordination number and stereochemistry of complexes – Applications of Lanthanide complexes as NMR shift reagents and MRI contrasting agents Actinides:- electronic structure – oxidation states – actinide contraction – spectral and magnetic properties in comparison with those of lanthanides and d-block elements. Trans actinide elements, IUPAC nomenclature – periodicity of trans actinide elements

UNIT – III	**ORGANOMETALLIC CHEMISTRY**	**18 Hours**

Introduction: Synthesis, reactions and applications of BuLi, Grignard, organoaluminum and organocopper reagents, 18 electron rule: counting methods and ligand contributions and explanation from MO theory. Hapto ligands with hapticity from 2-8, Davies-Green-Mingos (DGM) rules. Spectator ligands : Phosphines and NHC's: classification and properties.(Dewar- Chatt-Duncanson and mcp models) of metal alkene complexes. Reaction of metal bound alkene (the concept of Umpolung). Synthesis properties and chemical behavior of Fischer carbene and Schrock carbene complexes. Tebbe, Grubbs and Petasis reagents. Synthesis, structure and bonding of allyl, 1,3 butadiene metal complexes and ferrocene, Cobaltocene. Reactions – oxidative addition and reductive

elimination. σ-bond meta thesis. (1,1) and (1,2) migratory insertion reactions. Catalysis by organometallic compounds (eg: Fischer – Tropsch synthesis, alkene hydrogenation (Wilkinson's Synthesis), hydroformylation (Wacker process), Monsantoacetic acid process), Vaska's Complex and its use .

UNIT – IV	BIO INORGANIC CHEMISTRY	18 Hours

Metal ions in biological systems, Biochemistry of iron: Iron storage and transport. Ferritin and transferrin. Mechanism of biological nitrogen fixation, Structure and function of Nitrogenase (Fe-Mo and Fe protein) enzyme. Metal complexes in transmission of energy-chlorophylls. photosystems I and II in cleavage of water, model systems. Oxygen Transport - Haemoglobin and myoglobin. Nature of haeme-dioxygen binding. Cooperativity in haemoglobin. Non-haem proteins for O_2 transport-hemerythrin and haemocyanins,. Electron transfer proteins-cytochromes, iron-sulphur proteins (Bacterial Ferredoxins, Rubredoxin). Metalloproteins as enzymes– carboxy peptidase, carbonic anhydrase, alcohol dehydrogenase, superoxide dismutase -Structure and Mode of Action, Biomineralization Process. Therapeutic uses of Metals- Metal complexes in cancer therapy, rheumatoid arthritis, imaging agents and chelation therapy

REFERENCES

1. Alan G Sharp – Inorganic chemistry third edition, Pearson
2. J E Huheey, E A Keiter and R L Keiter, Inorganic chemistry principles of structure and reactivity, Pearson education
3. D F Shriver and P W Atkins, Inorganic Chemistry, Oxford University Press
4. Sathya prakash, G D Tuli, S K Basu and R D Madan, Advanced inorganic chemistry Volume II, S Chand Publication
5. Cotton, Wilkinson, Bachmann, Advanced inorganic chemistry, Wiley India Pvt Ltd
6. B Douglas D MeDaniel and J Alexander, Concepts and models of inorganic chemistry 3rd edition, John Wiley and Sons Inc
7. S J Lippard and J M Berg, Principles of bioinorganic chemistry, University Books California
8. David E Fenton, Bio coordination chemistry, Oxford University Press
9. I Bertni, H B Grey, S J Lippard and J S Valentine, Bio inorganic chemistry, Viva Books Pvt Ltd, New Delhi
10. DMP Mingo's Essential Trends in inorganic chemistry, Oxford University Press
11. K Hussain Reddy Bioinorganic chemistry New age international
12. Indrajith Kumar, Organometallic compounds, Pragati Prakashan Meerut
13. R C Melhotra and A Singh, Organometallic Chemistry, New age international

14. M.N. Hughes: Inorganic Chemistry of Biological Processes, (2ndedn.) Wiley, 1988.
15. K. Hussain Reddy, Bioinorganic Chemistry - New Age International Ltd. (2003).
16. R.W. Hay, Bioinorganic Chemistry - Ellis Horwood Ltd., (1984) 6. Asim K Das, Bioinorganic chemistry, Books & Allied (P) Ltd.
17. Gupta, B.D, Elias, A J; Basic Organometallic Chemistry, Concepts, syntheses and applications, 2nd edn, Universities Press, 2013.
18. Organometallics, Elschenbroich,Ch, 3 rd edn, Wiley VCH, 1989.
19. Organometallics and catalysis An introduction. Bochmann, M, 1st edn, Oxford, 2014
20. The organometallic chemistry of the transition metals, Crabtree R H, 6th edn, Wiley, 2014.
21. Organotransition metal chemistry: From bonding to catalysis, Hartwig, J.F, 1st edn, University science books, 2010.

MSCHD03C13: ORGANIC CHEMISTRY – III

Credit 4		**Time : 72 Hours**

Course Outcomes: After the completion of the course, the learners should be able to

CO1 :Understand the basics UV-Visible spectroscopy
CO2: Study the applications of electronic and IR spectroscopy in simple organic molecules.
CO3: Predict the structure of organic molecules using NMR spectroscopy
CO4: Differentiate the principle of HNMR and 13C NMR spectroscopy
CO5: Understand the basic principle of Mass spectroscopy and formulate methods to identify organic molecules using this technique
CO6: Elucidate and analyse the structure of different heterocyclic compounds and biomolecules

Course Content

UNIT I	**ELECTRONIC AND IR SPECTROSCOPY**	**18 Hours**

Colour and light absorption – the chromophore concepts – theory of electronic spectroscopy laws of light absorption – Beer-Lambertz law – solvents and solutions – effect of solvent polarity on UV absorption – electronic transition in enes, enones and arenes, Woodward Fieser rule Empirical rules for calculating λmax of dienes, enones and benzene derivatives. instrumentation and sampling.

IR spectroscopy – factors influencing vibrational frequencies – Conjugation, coupling, electronic, steric, ring strain and hydrogen bonding. principles of characteristics frequency in IR- application of IR – identity by finger printing – identification of functional groups and other structural features by IR – Hydrogen bonding and IR bands – Instrumentation and sampling techniques – FTIR and its instrumentation.

UNIT II	**NMR SPECTROSCOPY IN ORGANIC CHEMISTRY**	**18 Hours**

1HNMR: Chemical shift, factors influencing chemical shift, electronegativity, shielding and deshielding, van der Walls deshielding, anisotropic effect, magnetic anisotropy, H-bonding, diamagnetic and paramagnetic anisotropies. Chemical shift values of protons in common organic compounds, chemical, magnetic and stereochemical equivalence. Spin – spin coupling, types of coupling, coupling constant, factors influencing coupling constant, – analysis of 1st order spectra, spectral interpretation using actual spectra taken from standard texts . Simplification of NMR spectra use of high field NMR – shift reagents, chemical exchange and double resonance – NOE spectra, heteronuclear coupling. Introduction to COSY, HMBC, HMQC spectra.

13C NMR: General considerations, comparison with PMR, factors influencing carbon chemical shifts, carbon chemical shifts and structure-saturated aliphatics, unsaturated aliphatics, carbonyls, and aromatics. Off-resonance and noise decoupled spectra, Introduction to DEPT, INEPT, INADEQUATE.

UNIT III	**ORGANIC MASS SPECTROSCOPY**	**18 Hours**

Instrumentation – EI, CA, FAB, Electro spray and MALDI ion sources – magnetic high resolution (double focusing), TOF and Quadropole mass analysers – isotope abundance - molecular ion – molecular mass from molecular ion – meta stable ion – significance of meta stable ion – fragmentation process – basic fragmentation types and rule – factors influencing fragmentation – fragmentation associated with functional groups – alkanes, alkyne, halides, alcohols, ethers, carbonyl compounds, carboxylic acids, amides – characteristic fragmentation modes and Mc Lafferty rearrangement –GCMS, LCMS.

UNIT IV	**HETEROCYCLICS AND BIOMOLECULES**	**18 Hours**

Nomenclature of heterocycles, replacement and systematic nomenclature, Hantzsch-Widman system for monocyclic compounds. Synthesis and reactions of the following four membered heterocycles – oxitanes, azetidines and thietanes; five membered heterocylces – imidazoles, pyrazolines, six membered heterocycles –pyrimidines and pyrazines; seven membered heterocycles – azepines, oxepines and thiepines – fused heterocycles; indole, quinoline, isoquinoline and coumarins.

Steroids: Classification, structure and structural elucidation of cholesterol, conversion of cholesterol to progesterone, androsterone and testosterone. Structure, synthesis and biological activity of testosterone and androsterone, estrone, progesterone.

REFERENCES

1. W Kemp, Organic spectroscopy, Palgrave
2. J March, Advanced organic chemistry, Wiley
3. R O C Norman and A Coxon, Modern synthetic reaction, Chapman and Hill
4. M B Smith, Organic synthesis, McGraw Hill
5. R K Bansal, Synthetic applications in organic chemistry, Narosa

6. Robert M Silverstein, Francis X. Webster and David Kiemle, Spectrometric identification of organic compounds, Wiley 2005
7. Donald L Pavia, Gary M Lampman, George S Kriz and James R Vyvyan, Spectroscopy, Cengage Learning
8. RATAN Kumar Kar, Applications of redox and reagents in organic synthesis, New Central Book Agency
9. J Jouly and G Smith, Heterocyclic chemistry, Van-Nostrand, ELBS
10. Acheson, An introductory to heterocyclic compounds, Wiley-Eastern
11. Ahluwalia and Parashar, Heterocyclic and carbocyclic chemistry, Ane Books
12. Jagadanba Singh and Yadav, Oragnic synthesis, Pragati Prakashan Meerut
13. S K gosh, Advance general organic chemistry part 1 and 11, New central book

SEMESTER – III
MSCHD03C14: PHYSICAL CHEMISTRY – III

Credit 4		Time: 72 Hours

Course Outcomes: After the completion of the course, the learners should be able to

CO 1: To get an understanding of kinetic aspects of chemical reactions.
CO 2: To infer kinetic approach of Catalysis.
CO 3: To get a knowledge on surface chemistry and different surface catalysed reactions.
CO 4: To identify the colloidal system emphasizing on its stability and properties

Course Content

UNIT- I	**REACTION KINETICS**	**18 Hours**

Review of basic principles: Complex reactions- Reversible, parallel, consecutive and branching reactions- Principles of microscopic reversibility. Theories of reaction rate- collision theory–steric factor-potential energy surfaces- transition state theory- Eyring equation comparison of two theories- Thermodynamic formulation of reaction rates- significance of $\Delta G^{\#}$, $\Delta H^{\#}$ and $\Delta S^{\#}$ volume of activation- Effect of pressure and volume on the velocity gas reaction–Unimolecular reaction- Lindmann, Hinshelwood mechanism and RRK- RRKM theories- Fast reaction–relaxation, flow method-flash photolysis –Magnetic and Resonance method. Theoretical calculation of energy of activation.

UNIT – II	**KINETICS AND CATALYSIS**	**18 Hours**

Chain reaction–stationary and non-stationary chain- explosion and explosion limits-free radical and chain reaction- steady state treatment- kinetics of H_2-CI_2 and H_2-Br_2-decomposition of acetaldehyde- Rice Herzfeld mechanism- Branching chain-H_2O_2 reaction-Semenov Hinshelwood mechanism of explosive reaction. Acid – base catalysis-specific and general catalysis-prototropic and protolytic mechanism- examples-Acidity function. Enzyme catalysis-Michaelis-Menten equation derivation- effect of pH and temperature. Reaction in solution- Factors determining reaction rates in solution–

Effect of pressure-dielectric constant-ionic strength-cage effect-Bronsted- Bjerrum equation-Primary and secondary kinetic salt effect-Influence of solvent on reaction rate-Hammet & Taftequation.

UNIT – III	SURFACE CHEMISTRY	18 Hours

Thermodynamics of surfaces - surface excess –Gibbs adsorption equation and its verification - surfactants and micelles – surface film- surface pressure- Langmuir film balance-and surface potential - Application of Low energy electron-Diffraction and photoelectron spectroscopy- ESCA and Auger Spectroscopy to the study of surfaces. Adsorption -Different types of adsorption isotherms Langmuir adsorption isotherm -BET theory – Measurement of surface area of solids using Langmuir and BET isotherms. Heat of adsorption- and determination of heat of adsorption- Isosteric heat of adsorption Langmuir adsorption isotherm applied to rate laws for surface catalyzed reaction-Langmiur-Hinshel wood -The Eley-Rideal mechanism –flash desorption. Super hydrophobic surfaces- application.

UNIT – IV	COLLOIDS	18 Hours

Structure and stability of colloids: Origin of charge- The electrical double layer--zeta potential(derivation)-importance of zeta potential - factors affecting zeta potential – Factors contributing to stability of colloids. Electro kinetic phenomena- Electrophoresis-electro osmosis-sedimentation potential- streaming potential. Measurement of zeta potential-using sedimentation potential- streaming potential. Micelle-structure of Micelle- CMC- Factors affecting CMC Donnan membrane equilibrium-Macro molecules-different averages-Methods of molecular mass determination–Osmotic method- sedimentation methods -light scattering methods. Macromolecular dynamics- diffusion coefficient and molecular size determination from diffusion co-efficient.

REFERENCES

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3. J. Rajaram and J.C. Kuriacose- “Kinetics and Mechanism of chemical transformations”-Macmillan India Ltd

4. Alberty and Silbey-“Physical chemistry”-Wiley

5. G.K.Vemulappaly -“Physical chemistry”-Prentice Hall of India

6. P.W. Atkins-“Physical chemistry”-Oxford University press

7. A.W.Adamson-“Thephysicalchemistryofsurfaces”-4th edition-Wiley1982

8. Alexander and Johnson-“Colloid science”-Oxford University Press

9. Gavariker-“Polymer science”–New age International publishers

10. K.J. Laidler- John. H. Melser-“Physical chemistry”-CBS

11. Gorgen M Barrow, "Physical Chemistry", 5th edn Tata McGraw-Hill

SEMESTER – III
OPEN ELECTIVE I
MSCHD03O01: FOOD CHEMISTRY

Credit 4		**Time : 72 Hours**

Course Outcomes: After the completion of the course, the learners should be able to

CO1: Understanding fundamentals of food chemistry

CO 2: To acquire knowledge in Food Additives, Preservatives, and Contaminants

CO3: To gain concepts on food composition and nutritional aspects

CO4: Familiarity with analytical methods and Nanotechnology in food science

Course Content

UNIT–I	**CHEMISTRY OF FOOD: INGREDIENTS AND FLAVOR ENHANCERS**	**18 Hours**

Introduction, Historical development of food chemistry. Food Constituents-Carbohydrates-classification and physical properties, changes of carbohydrates on cooking. Lipids-occurrence in food and composition, fats and oils, Hydrogenation, Rancidity, reversion, rendering, extraction and refining. enzymes- classification and properties, vitamins-fat and water soluble, peptides, amino acids and protein-physical properties. Protein sources, Protein denaturation. Determination of proteins in food. Minerals obtained from food. Synthetic and natural Aroma compounds, Aroma value and threshold value. Sweeteners-Saccharin, Cyclamate, Aspartame. MSG as flavouring enhancer.

UNIT–II	**CHEMISTRY OF FOOD: ADDITIVES, PRESERVATIVES, AND CONTAMINATION**	**18 Hours**

Chemical Aspects of Additives, and Preservatives. Categories of Food Colours. Water Soluble and fat-soluble Synthetic Colours. Classification of Food Colorants-Natural and synthetic colorants. Classification of Food Additives. Food Spoilage and Preservation: Causes of Spoilage, Principle of Food Preservation. Factors Affecting Chemical Preservation, Classification of Chemical Preservatives, Types of Chemical Preservatives, Natural Chemical Preservatives, Methods of Food Preservation. Advantages and disadvantages of Food Additives and Preservatives. Effects and safety of Food Additives and Food Preservatives. History and types of Food Adulteration: Intentional, Incidental and Metallic Adulteration. Food contamination-Toxic trace elements and compounds.

UNIT–III	**CHEMICAL COMPOSITION OF FOOD**	**18 Hours**

	AND NUTRITIONAL ASPECTS	

Chemical Composition of Food and Food Commodities-Beverages and Drinks, Cereals and Their Products, Eggs and Egg Products, Edible Fats and Oils, Fish and Fishery Products, Meat and Meat Products, Milk and Milk Products. Composition of chemicals in vegetables and fruits. Compositions of tea and coffee. Composition of Honey and artificial honey. Raw materials and brewing process of beverages. Nutritional and Toxicological Aspects of the Chemical Changes of Food Components and Nutrients During Drying, During Freezing, During Heating and Cooking. Nutritional Values of Fermented Foods, Nutritional Quality of Fermented Vegetables and Fruits

UNIT – IV	**ANALYTICAL METHODS AND NANOTECHNOLOGY IN FOOD**	**18 Hours**

Chemical Analysis of Food Components: Classical Wet Chemistry Methods, Sampling and Sample Preparation, Instrumental Food Analysis. Analysis of drinking water. Standards for mineral water. An Introduction to Food Nanotechnology, Applications of Nanotechnology in Developing Biosensors for Food Safety, Advances of Nanomaterials for Food Processing. Bioactive Ingredients in Functional Foods and Nutraceuticals. Bioactive Substances of Plant Origin, Animal Origin, Microbial Origin and Synthetic Bioactive Substances.

REFERENCES

1. Mousumi Sen, Food Chemistry: The Role of Additives, Preservatives and Adulteration
2. Peter C. K. Cheung, Bhavbhuti M. Mehta, Handbook of Food Chemistry.
3. Owen R Fennema, Food Chemistry
4. H.D. Belitz, W. Grosch, P. Schieberle, Food Chemistry
5. Lillian Hoagland Meyer, Food Chemistry, CBS Publishers and Distributors
6. HD Belitz, W. Grosch, P Schieberle, Food Chemistry, Springer 4th Edn.
7. Matthew Hartings, Chemistry in your Kitchen, Royal Society of Chemistry
8. J. R. Hanson, Chemistry in the Kitchen Garden, RSC Publishing.

SEMESTER – III

OPEN ELECTIVE I
MSCHD03O02: ENVIRONMENTAL CHEMISTRY AND DISASTER MANAGEMENT

Credits 4		**Time : 72 Hours**

Course Outcomes: After the completion of the course, the learners should be able to

CO1 :To infer the chemical aspects of Atmosphere and Environmental pollution
CO2 : To survey the various analytical measuring methods of pollution monitoring
CO3: To explain the basic terminologies related to disaster and disaster management.
CO4: To identify, classify and assess laboratory accidents
CO5: To describe chemical hazards in laboratories, chemical safety and disposal of chemical wastes

Course Content

UNIT – I	**ENVIRONMENTAL AND ATMOSPHERIC POLLUTION**	**18 Hours**

Components of environment. Factors effecting the environment – segments of environmental. Atmosphere – composition and structure. Soil – composition and process of soil formation. Hydrosphere – sea water and river water composition. Environmental pollution – pollutant definition – origin, classification and types of pollution. Air pollution – sources (industrial, automobiles) – effect of SO_2, NO_X, CO, H_2S, smoke, hydrocarbons on human and plant systems. Cause and consequence of acid rain, green house effect, ozone depletion and photochemical smog. Air pollution control method. Air pollution accident – Bhopal tragedy

UNIT – II	**SOIL, WATER, THERMAL AND RADIOACTIVE POLLUTION AND INSTRUMENTAL METHODS IN CHEMICAL ANALYSIS**	18 Hours

Soil pollution sources – effect of fertilizers as soil utilization and agricultural work, pesticide and herbicides. Control methods. Water pollution – sources, effect of pollutants – oxygen deficiency, eutrophication. Water quality criteria for industrial and domestic use. Sewage treatment – industrial waste water treatment, experimental determination DO, COD, and BOD. ISI standard of drinking water. Thermal and radioactive pollution. Sources and control of thermal pollution. Sources and effects of radioactive pollution

A brief study i) AAS, ii) X-ray fluorescence, iii) gas chromatography and iv) ion selective electrodes

UNIT – III	**INTRODUCTION TO DISASTERS AND DISASTER MANAGEMENT**	**18 Hours**

Concept and terminologies - Hazard, Disaster, Risk and Vulnerability; Resilience; Classification-

Geological, Climate related, Biological, Technological, Environmental and Anthropogenic disasters, pandemics and epidemics; Disaster management cycle:-, Prevention, Mitigation, Preparedness, Response, Recovery and Reconstruction; Natural Disasters, Natural Disasters Induced by Human Interventions, Exclusively Human-made Disasters; Nuclear disaster (Chernobyl disaster and Fukushima nuclear disaster) and their management; Chemical disasters (Bhopal gas tragedy) and oil spills (deepwater horizon oil spill), Role of chemists in Disaster Management; Risk analysis, Risk assessment and Risk reduction (Do's and Don'ts in landslide, earthquake, cyclone, flood, tsunami, forest fire, fire accidents); Key aspects of Disaster Management Act 2005; Stakeholders, their roles and organizational structure (from national to district level), Disaster vulnerability profile of Kerala.

UNIT – IV	**LABORATORY HYGIENE AND SAFETY**	**18 Hours**

Awareness of Material Safety Data Sheet (MSDS). Hazardous Symbol (Physical, Chemical, Environmental and Health), storage, handling and transportation of hazardous materials; Lab accidents and safety measures; Fire safety in educational institutions and factories; Flash point and fire point for fuels; Simple first aids: Electric shocks, fire accidents, burn by chemicals, cut by glass and inhalation of poisonous gases (demo of cardiopulmonary resuscitation)- Accidents due to acids and alkalis - Burns due to phenol and bromine; Chemical decontamination, Disposal of sodium, mercury and other toxic wastes; R & S Phrases and H & P statements (elementary idea only); Safe laboratory practices and Lab safety signs;. Personal protective equipment (PPE); Design of a safe chemical laboratory.

REFERENCES

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26. S R Manjunatha and Manish Rathi, Environmental Chemical Hazards, Cyber Tech Publications
27. Emergency Response Guidebook published by IUPAC
28. Mohan Kanda, Disaster management in India- Evolution of Institutional Arrangements and Operational Strategies, Bio-green books
29. Nidhi Gauba Dhawan and Ambrina Sardar Khan, Disaster Management and Preparedness, CBS Publishers & Distributors
30. Geeta Singh, Climate change and Disaster management, Shivalik Prakashan
31. Benjamin R Sveinbjornsson and Sveinbjorn Gizurarson, Handbook for Laboratory Safety, Elsevier
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33. Central Motor Vehicle Rules India- 1989, Chapter 5
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35. S. Modh, Managing Natural Disasters, Mac Millan publishers India LTD., 2010.

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SEMESTER III
OPEN ELECTIVE I
MSCHD03O03 : INTER DISCIPLINARY TOPICS AND INSTRUMENTATION TECHNIQUES

Credits: 4		**Time :72Hours**

Course Outcomes: After the completion of the course, the learners should be able to

CO 1: To get knowledge about Supramolecular Chemistry
CO 2: To know the Principle of Green Chemistry and methods of Green Synthesis
CO 3: To get an understanding about Nano Science and Technology
CO 4: To be able to explain Electron Spin Resonance Spectra
CO 5: To be able to explain Mossbauer Spectra

Course Content

UNIT – I	**SUPRA MOLECULAR CHEMISTRY**	**18 Hours**

Introduction to supra molecular chemistry, molecular forces, common supra molecules, experimental techniques in supra molecular chemistry, host/guest chemistry, molecular recognition – molecular receptors for different types of molecules including arisonic substrates, design and synthesis of co receptor molecule and multiple recognition – amphiphile organization, supra molecular design strategy and nanotechnology. Supra molecular devices. Supra molecular photochemistry, supra molecular electronic, ionic and switching devices.

UNIT – II	**GREEN CHEMISTRY**	**18 Hours**

Introduction, the need of green chemistry, principles of green chemistry, planning of green synthesis, tools of green chemistry, green reactions, Aldol condensation, Cannizaro reaction and Grignard reaction – comparison of above with classical reactions – green preparations, applications – phase transfer catalyst – introduction to microwave organic synthesis – applications: environmental, solvents, time and energy benefits

UNIT – III	**NANOSCIENCE AND TECHNOLOGY**	**18 Hours**

Introduction – nanostructures,: tubes, fibers, bricks and building block, nanostructure formation:

lithography, self-assembly, molecular synthesis, crystal growth and polymerization, measurement of nanostructure: spectroscopy, microscopy and electrochemistry, material study: nano composites, consumer goods, smart materials, applications to various fields: optics, telecommunication, electronic, digital technology, and environmental, biomedical applications; diagnosis, mapping of genes, drug delivery, biomimetics, quantum dots

UNIT – IV	INSTRUMENTATION TECHNIQUES	18 Hours

Scattering methods – Nephelometry and turbidimetry – effects of concentration, particle size and wavelength of scattering, instrumentation and application. Electron spin resonance spectroscopy – basic principles – hyperfine coupling – the g values – isotropic and anisotropic hyperfine coupling constants – zero field splitting and Kramer's degeneracy – application to simple inorganic and organic free radicals and to inorganic complexes. Mossbauer spectroscopy; The Mossbauer effect – chemical isomer shift – Doppler effect – quadrupole interactions – measurement techniques and spectrum display – application to the study of Fe^{2+} and Fe^{3+}

REFERENCES

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2. P T Anastas and J C Warner Green Chemistry Oxford
3. G A Ozin, A C Arsenault, Nano chemistry RSC
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5. V S Muralidharan, A Subramania, Nano science and technology, Ane books
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SEMESTER IV

ELECTIVE PAPER II

MSCHD04E01 - INTRODUCTION TO DRUG CHEMISTRY

Credits: 4		Time :72 Hours

Course Outcomes: After the completion of the course, the learners should be able to

CO1. Understand the chemical and biological basis of action of drugs

CO2. Describe action of drugs through suitable examples and combine the principles of pharmacokinetics and pharmacodynamics to understand the mechanism of action of drugs

CO3. Understand the concepts of toxicity and illustrate different methods of biotransformations of drugs including phase I and phase II transformations with suitable examples of drug molecules

CO4. Compare the mechanism of action and therapeutical use of various anti-infective agents, analgesics, anti-pyretics, anti-inflammatory drugs and therapeutic agents with suitable examples

CO5. Synthesize the drugs -pethidine , phenyl butazone, diclophenac and codeine.

Course Content

UNIT -I	**PHARMACOLOGY**	**18 Hours**

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.

Structure activity relationship, Binding interactions, Functional groups as binding groups, Concept and definition of pharmacophore

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.

Pharmacodynamic principles : Examples of agonists, allosteric modulators, Antagonists, Partial agonists, Inverse agonists, Desensitization and sensitization, Tolerance and dependence, Affinity, efficacy and potency.

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

UNIT -II	**TOXICOLOGY AND BIOTRANSFORMATIONS**	**18 Hours**

General concepts of toxicity, Acute, subacute & chronic toxicity tests, teratogenicity & carcinogenicity, LD50, ED50, MIC- anti infectives, habituation & addiction.

Biotransformation of Drugs, factors affecting biotransformation, site of biotransformation, 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 - Glucuronidation, sulfation, conjugation with glutathione, acetylation methylation- illustrate with suitable drug molecules.

UNIT -III	**ANTI-INFECTIVE AGENTS**	**18 Hours**

Antibiotics/ Antibacterial Agents- Classification, mechanism of action and therapeutic uses-

penicillin, cephalosporins, Quinolones, Aminoglycosides, Carbapenems, macrolide and others. Antibiotic resistance mechanism and implications in therapeutics.

Synthetic studies of: Penicillin V, Streptomycin, Ciprofloxacin

Sulphonamides- structure, chemistry, SAR and mechanism of action of Sulfadiazine, sulfamethoxole, sulfones.

Antifungal agents: study of the following- Amphotericin B, ketoconazole, clotrimazole.

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

Antiviral agents: Antiviral drugs- mode of action and therapeutic uses, Chemistry and mechanism of action of- amatidine, ribavirin.

Antimalarials : 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- Qunine sulphate, Chloroquine and proguanil.

Chemotherapy of Tuberculosis: First line Drugs and second line drugs- chemistry Pharmacology. The problem of MDR tuberculosis.

UNIT -IV	**ANALGESICS, ANTIPYRETICS & ANTI-INFLAMMATORY DRUGS**	**18 Hours**

Analgesics- Different types of analgesics-Mechanism of action of Different types of analgesics.

Narcotic analgesics - morphine and codeine, phenyl (ethyl) piperidines

Antipyretics and NSAIDs: Basic idea of COX I & II inhibitors, salicylates - aspirin, p- aminophenol derivatives-paracetamol, phenacetin, anthranilic acid derivatives – flufenamic acid, arylacetic /propionic acid derivatives (ibuprofen, ketoprofen and diclofenac

Anti-inflammatory agents- Non steroidal anti inflammatory agents - Sulindac, Naproxen

Novel Analgesics: Raxatrigine (Structure only).

Synthesis of the following drugs- pethidine, phenyl butazone, diclofenac, Codeine.

REFERENCES

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SEMESTER IV

ELECTIVE PAPER II

MSCHD04E02 - BIOCHEMISTRY AND BIOPHYSICAL CHEMISTRY

Credits 4		**Time : 72 Hours**

Course Outcomes: After the completion of the course, the learners should be able to

CO1. Classify proteins based on their structure and functions

CO2. Design the mechanism and kinetic models of different types of enzymatic reactions, including reactions of coenzyme and describe the biotechnological applications of enzymes in drug design

CO3. Relate the functions and mode of actions of various hormones

CO4. Describe the transfer and utilization of energy in biological system through the metabolism of carbohydrates, lipids and proteins

CO5. Apply the biological importance of p^H and buffer solutions in pharmaceutical and biological systems

Course Content

UNIT -I	**AMINO ACIDS AND PROTEINS**	**18 Hours**

Physicochemical properties, configuration and optical properties of amino acids. Purification of proteins and amino acids, sequence determination. Solid phase peptide synthesis. Structural and functional classification of proteins. Primary, Secondary Tertiary and Quaternary structure of Proteins. Protein folding, three dimensional structure of proteins. Important proteins- fibrous and globular proteins- examples (keratin, collagen, hemoglobin and myoglobin).

UNIT -II	ENZYMES	18 Hours

Enzymes; Classification, Mechanism of enzymatic reactions, kinetics of enzymatic reactions, Michaelis Menton model, Significance of Kmax and Vmax. Inhibition of enzymatic reactions. Kinetics of competitive and non-competitive Inhibition. Allosteric enzymes, Mechanism of enzymatic catalysis by Lysozyme and carboxy peptidase, Zymogens.

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. Coenzyme - A, and Thiamine pyrophosphate.

Biotechnological Application of Enzymes; Large scale production and purification of enzymes, Techniques and method of immobilization of enzymes, effect of immobilization on enzyme activity, Application of immobilized enzymes, use of enzymes as targets for drug design.

UNIT -III	NUCLEIC ACIDS AND HORMONES	18 Hours

Nucleic acids: Nucleic acid bases, Nucleosides, nucleotides, structure of DNA, RNA and its classification.

Replication of DNA, transcription, translation and Protein Biosynthesis.

Restriction enzymes. 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.

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 -IV	BIOLOGICAL OXIDATION AND METABOLISM	18 Hours

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.

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

Protein and amino acid metabolism: Oxidative deamination and trans amination reactions, Urea

formation- ornithine cycle.

Buffer systems - Biological relevance of pH and pKa, determination of pKa of weak acid -Buffer in pharmaceutical and biological systems, pH, the buffer equation (Henderson Hesselbach), Buffer calculations. Three important buffer systems in human body (cytosol and blood). Buffer capacity, osmotic pressure and tonicity, Pharmaceutical buffers, preparations of pharmaceutical buffer solutions.

REFERENCES

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SEMESTER IV

ELECTIVE PAPER II

MSCHD04E03 - INTRODUCTION TO COMPUTATIONAL CHEMISTRY & COMPUTATIONAL DRUG DESIGN

Credits 4		Time : 72 Hours

Course Outcomes: After the completion of the course, the learners should be able to

CO1. Understand the basic principles and significance of computer aided drug discovery.

CO2. Practice the quantum chemical calculations to yield useful information such as electron densities, energies and other properties of the molecular system.

CO3. Investigate the electronic structure of any kind of many electron system by simulation method - density functional theory.

CO4. Define and choose basis sets to model molecular orbitals.

CO5. Design and sketch 2D molecules using computer softwares – ChemSketch and ChemDraw and visualize 3D molecules using softwares –Avogadro and GaussView.

CO6. Understand how modern drugs are developed using molecular modeling and docking techniques.

CO7. Apply cheminformatic and bioinformatic tools in drug design.

Course Content

UNIT -I	INTRODUCTION TO COMPUTATIONAL CHEMISTRY	18 Hours

Theory, computation & modeling – Definition of terms. Need of approximate methods in quantum mechanics. Computable Quantities – structure, potential energy surfaces and chemical properties. Cost & Efficiency – relative CPU time, software & hardware. Classification of computational methods.

ab initio Methods in Computational Chemistry -Review of Hartree – Fock method for atoms, SCF treatment of polyatomic molecules; Closed shell systems - restricted HF calculations; Open shell systems – ROHF and UHF calculations; The Roothan – Hall equations, Koopmans theorem, HF limit & electron correlation, Introduction to electron correlation (post -HF) methods: Møller Plesset Perturbation Theory, Configuration Interaction, Coupled Cluster and semi empirical methods (elementary idea only).

UNIT -II	DENSITY FUNCTIONAL METHODS AND BASIS SET APPROXIMATION	18 Hours

Introduction to density matrices, N-representability & V-representability problems, Hohenberg – Kohn theorems, Kohn-Sham orbitals, Exchange correlation functionals– Thomas-Fermi- Dirac model, Local density approximation, generalised gradient approximation, hybrid functional. Comparison between DFT and HF methods.

Basis Set Approximation - Hydrogen-like, Slater-type & Gaussian type basis functions, classification of basis sets – minimal, double zeta, triple zeta, split-valence, polarization & diffuse basis sets, contracted basis sets, Pople-style basis sets and their nomenclature, correlation consistent basis sets, basis set truncation error, effect of choice of method / basis set (model chemistries) on CPU time.

UNIT -III	QUANTUM CHEMICAL CALCULATIONS	18 Hours

Preparation of 2D molecules using ChemSketch and Chemdraw - Molecular editor and visualization in 3D using Avogadro / GaussView / McMolPlt / ChemCraft. Simple calculations using Gaussian / GAMESS / Turbomole / Orca quantum chemistry programme – The structure of an input file, Types of keywords, Specification of molecular geometry using (a) Cartesian coordinates and (b) Internal coordinates. The Z-matrix, Z- matrices of some simple molecules like H_2, H_2O, formaldehyde, ammonia and methanol etc. Calculation of single point energy – minimization of molecular structures by geometry optimization - characterizing stationary points – interpreting normal mode information – calculation of IR and Raman spectra - modeling thermochemistry .

UNIT IV	COMPUTATIONAL APPROACHES TO DRUG DESIGN AND DISCOVERY	18 Hours

General approach to discovery of new drugs - Drug Discovery Cycle, The Lead compound, Pharmacophore, database resources for drug discovery - chemical databases, physiochemical principles of drug action - ADME and Toxicity, Virtual Screening, Molecular Docking, Structure and Ligand Based Drug Designing. Structure comparison and overlays – identification of active conformations - Tools for Molecular Visualization and Analysis: RASMOL, PYMOL - Molecular Electrostatic Potentials - Molecular Modeling and Docking: Automated screening of databases for lead compounds - *De novo* drug design

REFERENCES:

1. C. J. Cramer, *Essentials of Computational Chemistry: Theories and models,* John Wiley & Sons 2002.
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6. I.N. Levine, *Quantum Chemistry*, 6th Edition, Pearson Education Inc., 2009.
7. P.W. Atkins & R.S. Friedman, *Molecular quantum mechanics*, 4th Edition, Oxford University Press, 2005.
8. W. Koch, M.C. Holthausen, *"A Chemist's Guide to Density Functional Theory"*, Wiley-VCH Verlag 2000.
9. D. Baxivanis and Foulette - Bioinformatics: A Practical Guide to the Analysis of Genes and Proteins, Wiely Indian Edition, 2001.
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SEMESTER IV

ELECTIVE PAPER III

MSCHD04E04 – ADVANCES IN DRUG CHEMISTRY AND DRUG DESIGN

Credits 4		**Time : 72 Hours**

Course Outcomes: After the completion of the course, the learners should be able to

CO1. Understand the basic principles of design and development of new drugs.

CO2. Incorporate computational techniques of virtual screening including both pharmacophore screening and structural based virtual screening (from database)

CO3. Develop relationship between physicochemical properties and biological activity of chemical substances and use this as a model for prediction of the activity of newly proposed lead molecules

CO4. Create large number of different but structurally similar molecules which can act as lead compounds by applying combinatorial chemistry and understand the process High Throughputs Screening (HTS)

CO5. Describe the mechanism of action and uses of different classes of drugs - antineoplastic drugs, drugs acting on autonomic nervous system and central nervous system.

Course Content		
UNIT -I	**DRUG DESIGN AND DEVELOPMENT**	**18 Hours**
Development of new drugs, procedures followed in drug design - Concept of lead compounds and lead modification & lead optimization- phytochemicals as lead compounds - Prodrugs and soft drugs. Functions and properties of prodrugs and its effect and significance with relation to pharmacological activity - Endogenous compounds as drugs -neurotransmitters, natural hormones - Peptidomemetics in drug design - SAR, factors affecting bioavailability, resonance and inductive effects, isosterism, bioisosterism – thermodynamics of biological systems. **Computer Aided Drug Design (CADD)** -Virtual screening- concept, drug likeness screening, focused screening libraries for lead identification, pharmacophore screening, and structure based virtual screening and application. Molecular modeling- introduction, molecular methods, Molecular mechanics, modeling ligands for known and unknown receptors. Docking studies - Machine Learning Approaches to Rational Drug Design		
UNIT -II	**QSAR AND COMBINATORIAL CHEMISTRY**	**18 Hours**
Introduction and perspectives and parameters involved in studies of QSAR - Types of QSAR models - Classification of parameters utilized in QSAR studies - Statistical concept of QSAR - Hansch model of QSAR - De Novo model of QSAR - Hammett and Taft model of QSAR equations - Applications of QSAR in drug design Combinatorial Chemistry Introduction - Combinatorial approaches - Peptide and small molecule libraries - Applications, methodology - Combinatorial Organic Synthesis - Assays and Screening of Combinatorial libraries - Introduction to High Throughputs Screening (HTS)		
UNIT -III	**DRUGS ACTING ON ANS**	**18 Hours**
Drugs acting on ANS-Introduction to autonomic nervous system and classification. Mechanism of action and uses of the following classes of drugs: Adrenergic agonists : oxymetazoline, salbutamol. Adrenergic blockers: α and β adreno-receptors, antagonists-ergot alkaloids- Pronethalol, propranolol, atenolol. Cholinergic stimulants: nicotinic and muscarinic receptors, acetyl choline. Cholinergic blockers: atropine. Nicotinic antagonists: Decamethonium and suxamethonium. Organo phosphorous		

compounds and nerve gases (Elementary idea only).

UNIT-IV	DRUGS ACTING ON CENTRAL NERVOUS SYSTEM AND ANTINEOPLASTIC DRUGS	18 hours

Pharmacology of the following classes of drugs -Hypnotics, sedatives and anxiolytic agents.

Anxiolytic agents-benzodiazepines, buspirone and meprobamate.

Anticonvulsants: Barbiturates- hydantoins, oxazolidinediones, succinimides and benzodiazepines.

Analeptics: xanthines, amphetamines, nikethamide and ethamivan.

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

Cancer chemotherapy - Role of alkylating agents, antimetabolites and folate antagonists in the treatment of cancer. Carcinolytic antibiotics and mitotic inhibitors - Plant derived drugs - vincristine, taxol - Hormones and their antagonists - Recent developments in cancer chemotherapy - immunological interventions.

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
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10. Computer aided Drug design, TJ PERUN7 CL Propst, Marcel& Dekker, 2007.
11. Introduction to Principles of Drug Design, Smith H J, Williams 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.

Medicinal Chemistry, Alex Gringauz, Wiley

SEMESTER IV

ELECTIVE PAPER III

MSCHD04E05: MEDICINAL CHEMISTRY

Credit 4		**Time : 72 Hours**

Course Outcomes: After the completion of the course, the learners should be able to

CO1. Understanding of drug classification and nomenclature

CO2. Knowledge of mechanisms of drug action and metabolism

CO3. To familiarize with medicinal compounds synthesis and applications

CO4. Attain concepts on antibiotics, antiseptics, analgesics and anesthetics

CO5. To understand the treatment of common diseases by drugs

Course Content

UNIT – I	**DRUG CLASSIFICATION, NOMENCLATURE, MECHANISM, AND METABOLISM**	**18 Hours**

Introduction: Nature and source of drugs – study of drugs – important terminologies in pharmaceutical chemistry

a) Classification and nomenclature of drugs: biological classification, chemical classification, classification of drugs according to commercial considerate, classification by lay public, nomenclature of drugs, some important heterocyclic systems and their nomenclature

b) Mechanism of drug action and metabolism of drugs: Introduction – mechanism of action of drug, mechanism of different types of drug action, metabolism of drugs, absorption of drugs, assay of drugs

UNIT – II	**ANTIBACTERIAL DRUGS , ANTISEPTIC AND DISINFECTANTS**	**18 Hours**

a) Antibacterial drugs: Sulpha drugs; sulphanilamides – properties of sulphanilamides, mechanism of action of sulfa drugs, sulphadiazine, sulphapyridine, cibazole, sulphafurazole, Prontosil – Antibiotics; classification of antibiotics, chloramphenical, pencillin, streptomycin, tetracycline, macrolides

b) Antiseptic and disinfectants: Phenols and its derivatives – halogen compounds –dyes – organic mercurials – formaldehyde and its derivatives – nitrofuran derivatives – cationic surface active agents

UNIT– III	**ANESTHETICS, ANALGESICS, ANTIPYRETIC,**	**18 Hours**

	AND ANTI-INFLAMMATORY AGENTS	

a) Anesthetics: General anesthetics – volatile general anesthetics; ether, chloroform, haloethane, trichloroethylene, ethyl chloride, nitrous oxide, cyclopropane – Intravenous anesthetics; thiopental sodium, methohexitone – local anesthetics; the esters, cocaine, benzocaine, procaine, amethocaine, proxy metacaine – the amides; lignocaine, cinchocaine

b) Analgesics, antipyretic, and anti-inflammatory agents: Narcotic analgesics – natural narcotic analgesics; morphene, heroin, apomorphine – synthetic narcotic analgesics; pethidine, morphinan, benzomorphan – non narcotic analgesics; salicylic acid derivatives, the paraminophenol, the pyrazole, indolyl and aryl acetic acid derivatives.

UNIT - IV	**CAUSES OF COMMON DISEASES AND THEIR TREATMENT BY DRUGS**	**18 Hours**

Insect borne disease and their treatment; malaria, filariasis, plague – air borne disease, their controls and treatment; diphtheria, wooping cough, influenza, measles, mumps, tuberculosis – water borne diseases; cholera, typhoid, dysentery –disorders of digestive systems – jaundice – disease of respiratory system; asthma – common disorder of nerve system; epilepsy – some common diseases; piles, leprosy – first aid for accidents – detection of hallucinogens and poisons - antidotes for poisoning

REFERENCES

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2. K D Tripathi, Essentials of medical pharmacology, 6th edtn, Jaypee
3. G Thomas, Medicinal chemistry an introduction, Wiley
4. G L Patrick, Introduction to medicinal chemistry, Oxford
5. A Kar, Medicinal chemistry, New age
6. D Sriram, P Yogeeswari, Medicinal chemistry, Pearson Education
7. G Thomas, Fundamentals of medicinal chemistry, Wiley
8. Padmaja Udayakumar, Medical Pharmacology
9. Ashuthosh Kar, Medicinal Chemistry
10. Kapoor & Gunn, Dispensing Pharmacy
11. B.M. Mithal, A Text Book of Forensic Pharmacy
12. Wilson & Gisvold, A Text Book of Organic and Pharmaceutical Chemistry
13. Gringauz A, Introduction to Medicinal Chemistry: How drugs act and why? John Wiley & Sons
14. VK Ahluwalia, M Chopra, Medicinal Chemistry, Ane Books India

SEMESTER IV

ELECTIVE PAPER III

MSCHD04E06: ADVANCES IN DRUG SYNTHESIS

Credits 4		**Time : 72 Hours**

Course Outcomes: After the completion of the course, the learners should be able to

CO 1 Understand the synthetic and stereochemical significance of different methods of functionalization of alkenes.

CO 2 Practice advanced synthetic methods in drug chemistry

CO 3 Design the strategies for combinatorial synthesis and synthesis of organic nanomaterials.

CO 4 Understand the significance of chiral synthesis and chiral building blocks in drug synthesis and drug delivery.

CO 5 Familiarize with various green techniques in drug synthesis.

CO 6 Understand the key concepts and features of click chemistry.

CO 7 Apply the principles of click chemistry in drug synthesis.

Course Content

UNIT-I	**FUNCTIONALIZATION OF ALKENES**	**18 Hours**

Hydroboration of alkenes – Mechanism, stereochemistry, factors affecting the product formation, applications in synthetic chemistry. Epoxidation – mechanism, different oxidizing agent used, factors affecting the rate, stereochemistry, Asymmetric synthesis of allylic alcohol and its epoxides and applications. Aziridination – Mechanism, asymmetric synthesis, applications. Dihydroxylation – dihydroxylation using OsO4, Mechanism, stereochemistry, asymmetric synthesis to obtain stereoselective products, applications. Amino-Hydroxylation – Mechanism, stereochemistry, asymmetric amino-hydroxylation and its application

UNIT-II	**ADVANCED SYNTHETIC METHODS IN ORGANIC CHEMISTRY**	**18 Hours**

Solid phase synthesis: Concept, resins, linkers, characterizations, examples. Peptide synthesis: Protected amino acids, coupling agents, strategies in synthesis with examples of peptide drugs and hormones. Disconnection Method: Concept, designing of synthesis, synthon and synthetic equivalents, functional group inter conversion (FGI), One group C-X and two group. C-X disconnections – Diels-Alder reaction, Protecting groups: Principle of protection of hydroxyl amino carboxylic and carbonyl groups. C-C one group and C-C two group disconnections -designing of synthesis of benzocaine (anesthetic)

Combinatorial synthesis: liquid phase and solid phase, deconvolution techniques, design of libraries

(these to be discussed with illustrative examples of combinatorial libraries).

Organic nanomaterials (Single molecular and molecular assemblies): Design, synthetic strategies, characterization and properties. Dendrimers, polymeric nanomaterials, carrier-systems for drug targeting (Overview only)

UNIT -III	CHIRAL SYNTHESIS	18 Hours

Introduction, concept and importance of chirality. Resolution of racemic mixtures. Stereoselective and stereospecific synthesis. Classification of Methods as first, second, third and fourth generation and their examples, reactions involved in chiral synthesis for compounds with one and two chiral centers. Examples of reactions of the above types useful in drug synthesis. Analytical methods in chiral synthesis.

Chiral building blocks for drugs synthesis via biotransformations – Anti cancer drug, modification of natural products- synthesis of taxane and epothilone, Anti inflammatory drugs- Profens- (s) ibuprofen and (s)- ketoprofen , Chiral medicines – Synthesis and applications of Aprepitant and Simvastatin . Drug delivery systems (Overview only)

UNIT-IV	GREEN TECHNIQUES IN ORGANIC SYNTHESIS	18 Hours

Green reagents: Dimethyl carbonate and Polymer supported reagents. Green catalysts: Acid basic catalysts and Oxidation catalysts. Aqueous phase reactions and photo chemical reactions. Applications of phase transfer catalyst and crown ethers in green chemistry. Microwave assisted reactions in water and organic solvents. Solvent free (solid state) reactions. Synthetic applications of ultrasound. Reactions in neutral Ionic liquids : Hydrogenation, Diels – Alder, Heck reaction, O - and N - alkylation and methylene insertion reaction, Supercritical Fluids (SCF) as media for chemical reactions .

Click chemistry – Concept and features. Cyclo-addition click reactions-azide- alkyne 1,3-dipolar cycloaddition(Huisgen cyclo-addition), Copper catalyzed azide-alkyne cyclo- addition. Thiol based click reactions- Thiol - ene radical click reaction, Thiol epoxide click reaction. Applications of click chemistry in drug synthesis – synthesis of enzyme inhibitors, fragment based drug discovery.

REFERENCES

1. R.A. Sheldon, Chirotechnology. Industrial Synthesis of Optically Active Compounds, Marcel Dekker, Inc., New York, 1993.
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3. F. A Carey and R.J. Sundberg, Advanced Organic Chemistry, 4th Edn., Parts A and B,

Springer

4. P. Larsen, T. Liljefors and U. Madsen Textbook of Drug Design and Discovery, CRC Press, New York
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7. S. R.Wilson and A. Czamik, Combinatorial Chemistry: Synthesis and Applications, Wiley, 2013
8. S. Warren Organic Synthesis, The disconnection Approach, 2nd Edn., Wiley
9. J. Clayden, Nick Greeves and Stuart Warren, Organic Chemsitry, 2nd Edn., Oxford University Press
10. E.J. Corey, The Logic of Chemical Synthesis, Wiley
11. K.C. Nicolou and E.J. Sorensen Classics in Total Synthesis, Wiley-VCH
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MSCHD03&04C15: INORGANIC CHEMISTRY PRACTICAL – II (3rd and 4th SEMESTER)		
Credit: 2		**Time: 108 Hours**

Course Outcomes: After the completion of the course, the learners should be able to

CO 1. Predict the methods for separation cations of a mixture

CO 2. Estimate metal ions present in a binary mixture following volumetric, gravimetric, and colorimetric methods

CO 3. Interpret data from an experiment, including constructing appropriate graphs and evaluating errors.

CO 4. Analyze alloys and detect the cations present

CO 5. Analyze trace metals using optical methods

CO 6. Synthesize and characterize nanoparticles by various methods.

Course content:

1) Quantitative separation of binary mixtures and estimation of components by

volumetric, gravimetric, colorimetric, and electroanalytical methods

Cu(II), Cr (VI), Ni(II), Fe(III), Mg(II), Al(III), Ca(II), Ba(II) and Zn(II)

2) Analysis of ores

a) Analysis of brass

b) Analysis of solder

3) Synthesis of any two of the following metal oxide nanomaterials and their characterization using X-ray, microscopic or spectrochemical methods.

- ZnO / TiO_2/ Co_3O_4/ $Co(OH)_2$ / NiO / FeO etc. (Any two)

[A minimum of 12 experiments to be recorded]

REFERENCES

1. G H Jeffrey, J Bassette, J Mendham and R C Denny, Vogel's textbook of quantitative inorganic analysis, ELBS Publication, London 1997
2. D M Adams and J B Raynor, Advanced practical inorganic chemistry, CRC Press, New York
3. W L Jolly, Preparative Inorganic reactions, Interscience Publishers, New York
4. Textbook of Nanoscience and Nanotechnology, 2012 McGraw Hill Education (India) Private Limited By T Pradeep
5. Springer Handbook of Nanomaterials, by Robert Vajtai
6. *Solution-Grown Zinc Oxide Nanowires, by Lori E. Greene, Benjamin D. Yuhas, Matt Law, David Zitoun, and Peidong Yang*, Inorg. Chem. 2006, 45, 7535−7543.*

MSCHD03&04C16: ORGANIC CHEMISTRY PRACTICAL – II

(3rd and 4th SEMESTER)

Credit: 2		**Time: 108 Hours**

Course Outcomes: After the completion of the course, the learners should be able to

CO 1. Develop lab skills in the extraction of natural compounds and qualitative analysis.

CO 2. Synthesize and purify organic compounds

CO 3. Develop skills in chromatographic techniques.

CO 4. Analyze, examine, and solve spectral data.

Course Contents:

1) Quantitative analysis and Extraction of natural products:

Estimation of the following

i) Phenol (Using bromate-bromide mixture)

ii) Aniline (Using bromate-bromide mixture)

iii) Reducing sugars (using Fehling solution)

iv) Iodine value of vegetable oil

v) Saponification of vegetable oil

vi) Estimation of ascorbic acid (Colorimetric method)

Extraction of natural compounds

i) Caffeine from tea leaves, and ii) Casein from milk

2) Two-stage preparation of organic compounds (minimum 5 compounds):

a) Preparation of p-nitroaniline from acetanilide:

Acetanilide----p-nitroacetanilide----p-nitroaniline

b) Preparation of Methyl orange from aniline:

Aniline---sulphanilic acid---methyl orange

c) Preparation of p-aminoazobenzene from aniline:

Aniline---diazoaminobenzene---p-aminoazobenzene

d) Preparation of m-nitroaniline from nitrobenzene:

Nitrobenzene---m-dinitrobenzene---m-nitroaniline

e) Preparation of Benzilic acid benzoin:

Benzoin----benzil----benzilic acid

f) Preparation of Benzanilide from benzophenone:

benzophenone---benzophenone oxime—benzanilide

g) Preparation of 2-phenyl indole from phenyl hydrazine:

Phenyl hydrazine----acetophenone phenyl hydrazone----2-phenyl indole

h) Preparation of caprolactam from cyclohexanone:

Cycohexanone----cyclohexanone oxime---Caprolactum

i) Preparation of m-nitrobenzoic acid from ethyl benzoate:

Ethyl benzoate----ethyl m-nitrobenzene----m-Nitrobenzoic acid

3) Chromatographic Techniques:

Practical application of TLC:

a) Identification of food colours, amino acids, and sugars.

b) Identify the compound from the mixture of hydrocarbon and acids. (Compare using Rf values with the standard values)

c) Column chromatography in separating the exact amount of a given mixture of o-nitroaniline and p-nitroaniline.

4) Spectral evaluation of organic compounds:

Solving spectral problems from the standard textbooks by providing IR, ^{1}H NMR, ^{13}C NMR, and Mass spectra. (15 simple compounds only) like Phenol, Benzophenone, Acetophenone, Acetone, benzoic acid, Benzamide, aniline, α-naphthol, glucose, benzaldehyde, aceldehyde etc….

[A minimum of 16 experiments to be recorded]

REFERENCES

1. A I Vogel, A Textbook of practical organic chemistry, Longmann

2. Elementary practical organic chemistry, part 3, quantitative organic analysis, Longmann

3. F G Mann and B C Saunders, Practical organic chemistry, Longman

4. PR Singh, DC Gupta & KS Bajpai, Experimental organic chemistry vol I&II

5. S Sadasivam and A Manickam, Biochemical methods, New Age International Publishers

6. J B Harbone, Phytochemical methods, Chapman and Hall, London

7. Joseph Sharma, Gunter Zweig, TLC and LC Analysis of international importance, Vol. VI and VII, Academic Press

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9. Organic Spectroscopy Principles, problems and their solutions, Jagadamba Singh and Jaya Singh, Pragati Edn.

10. Organic Spectroscopy Principles and Applications, Jag Mohan, Narosa Publishing House.

11. Organic Spectroscopy: Problems & Numericals, Dipti K Dodiya, Bluerose publishers.

12. Organic structures from spectra, 4th Edition, LD field, S Sternhell, JR Kalman, Wiley.

MSCHD03&04C17: PHYSICAL CHEMISTRY PRACTICAL – II (3^{rd} and 4^{th} SEMESTER)		
Credit: 2		**Time: 108 Hours**

Course Outcomes: After the completion of the course, the learners should be able to

CO 1. Experimentally analyze the concepts related to the kinetic aspects of chemical reactions- determination of concentration from graphs based on surface chemistry concepts

CO 2. Utilize stereochemical principles related to optical isomers to determine the concentration and kinetic parameters of specific reactions

CO 3. Apply UV-Visible spectroscopy to determine solution concentration, complex formation, equilibrium constant, metal ion concentration

CO 4. Perform basic spectral calculations and determination of specific parameters from UV-Visible spectroscopy and X-ray diffraction data

CO 5. Apply Computational chemistry to perform single-point energy calculation, geometry optimization, and Frontier orbital calculation at the HF level of theory

Course Content:

1) Chemical kinetics

Acid hydrolysis of ester (methyl acetate or ethyl acetate) – determination of the given acids.

Acid Hydrolysis of ester – determination of Arrhenius parameters

Saponification of ethyl acetate – determination of specific reaction rate, $K_2S_2O_8$, and KI system

Iodination of acetone in acid medium – determination of the order of reaction with respect to iodine and acetone

2) Adsorption

Verification of Freundlich and Langmuir adsorption isotherms – charcoal-acetic acid system

Determination of concentration of given acetic acid solution using the isotherms

The same experiment using a charcoal-oxalic acid system

3) Polarimetry

Determination of specific and molar optical rotations of glucose, fructose, and sucrose

Determination of the concentration of a glucose solution

Inversion of cane sugar in the Presence of HCl-Study of the Kinetics

Determination of the specific rate of the reaction

Determination of the concentration of HCl

4) Spectrophotometry

Verification of the Beer Lamberts law

Determination of equilibrium constants of acid-base indicators

Determination of concentration of a solution of $K_2Cr_2O_7$ (or $KMnO_4$)

Simultaneous determination of Mn and Cr in a solution of $KMnO_4$ and $K_2Cr_2O_7$

Investigation of complex formation between Fe(III) and thiocyanate

5) Spectral analysis calculations

Determination of band gap/ HOMO/LUMO from UV Vis/CV analysis

Determination of particle size/ Lattice parameters of Simple Cubic system from XRD

6) Computational Chemistry Calculations

Single point energy calculations of simple molecules like H_2O and NH_3 at the HF/3-21G level of theory.

The effect of the basis set on the single point energy of H_2O and NH_3 using the Hartree-Fock method (3-21G, 6-31G basis sets can be used).

Geometry optimization of molecules like H_2O, NH_3, HCHO & C_2H_4 at the HF/6-31G level of theory.

Computation of the energy of HOMO and LUMO of formaldehyde and ethylene at the. HF/6-31G level of theory.

Effect of substituent (F & Cl) on the geometric parameters (like C-C bond length) of ethylene at the HF/6-31G level of theory.

[A minimum of 16 experiments to be recorded]

REFERENCES

1. F Daniels and J H Mathews, Experimental physical chemistry, Longmann
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4. D P Shoemaker and C W Garland, Experimental physical chemistry, McGraw Hill
5. J B Yadav, Advanced practical physical chemistry, Goel Publishers
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7. V D Athawale Parul Mathur, Experimental physical chemistry, New Age International Publishers
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MODEL QUESTION PAPER
I Semester M.Sc. Degree (C.B.C.S.S. - OBE –Regular)
Examination, October 2023
(2023 Admission)
CHEMISTRY
MSCHD01C01: THEORETICAL CHEMISTRY I

Time: 3 hours **Max marks: 60**

SECTION A

Answer any 5 questions. Each question carries 3 mark.

(5×3 = 15 marks)

1. State Planck's radiation law
2. What is meant by normalisation of a wave function?
3. What are spherical harmonics? Are they mutually orthogonal?
4. State Variation theorem
5. Show that the ground state term symbol of H2 is $1\sum_g^+$
6. What is basis set?

SECTION B

Answer any 3 questions. Each question carries 6 marks. (3×6 = 18 marks)

7. What are eigen functions and eigen values ? Show that e^{ikx} is an eigen function of the momentum operator $\hat{P}x = i\hbar\, d/dx$. What is eigen value?
8. What will happen if the walls of the one dimensional box are suddenly removed? Explain
9. Explain spin orbit coupling and spin orbit coupling constant . Why is it very large in heavy elements?
10. What is meant by HFSCF procedure? Explain
11. What are the important problems faced in quantum mechanical calculations for many particles compared to a single particle? How it is overcome?

SECTION C

Answer any 3 questions. Each question carries 9 marks. (3×9 = 27 marks)

12. Give the postulates of quantum mechanics
13. Set up the Schrödinger wave equation of hydrogen atom in spherical polar coordinates. Separate the variables. How do the quantum numbers n,l and m emerge from the solution of three equations?
14. Obtain the normalized wave function and energy for a particle confined in a three dimensional box with lengths Lx, Ly and Lz. Evaluate the results
15. Give the Molecular Orbital (MO) treatment for the following molecules
    (i) Be_2 (ii) NO (iii) LiH
16. Setup the Huckel secular equation for cyclo butadiene , calculate the energies of the π orbitals and determine the delocalisation energy.

Model Question Paper

MSCHD01&02C05: INORGANIC CHEMISTRY PRACTICAL– I

Time: 6 Hours

Max Marks:40

1. You are given a mixture containing four cations at least two of which are those of rare metals. Find out the cations by a systematic procedure (14 Marks)
2. Determine the amount of calcium/nickel in the whole of the given solution. You are provided with 0.05M EDTA and AR zinc sulphate (12 Marks)
3. Prepare the complex marked (X) below and exhibit crude as well as recrystallized samples;
   a) Nickel (dimethyl glyoxime)
   b) Potassium trioxalatochromate (III)
   c) Tetraammonium copper (II)sulphate
   d) Hexamminecobalt (III) chloride
   e) Potassiumhexathiocyanato chromate(III) (6 Marks)

4. Write down the principle and procedure of the volumetric estimation of……. by ..……..... on a separate sheet of paper. (3 Marks)
5. Record (Minimum 16 Experiments) (5 Marks)

Model Question Paper

MSCHD01&02C06: ORGANIC CHEMISTRY PRACTICAL – I

Time: 6 Hours

Max Marks:40

1. Separate and suggest a suitable method for the separation of the components and analyze them systematically. Write the procedure for the separation and also the analysis of the components. Determine the physical constant of the components. Suggest and prepare a crystalline derivative for each component. Exhibit the components and derivatives properly labeled for inspection. (25 Marks)
2. Prepare any of the ( ) following compounds. Exhibit the crude and the recrystallized samples for inspection by examiners. Spot the TLC using both reactant and product and describe the chromatogram to the examiners.
   a) p-Bromoacetanilide from acetanilide
   b) p-Nitroacetanilide from acetanilide
   c) Benzanilide from aniline (6 Marks)
3. Write down the mechanism involved in the preparation of…….. (2 Marks)
4. Exhibit a minimum of two polymer samples for inspection. (2 Marks)
5. Record (5 Marks)

Model Question Paper
MSCHD01&02C07: PHYSICAL CHEMISTRY PRACTICAL – I

Time: 6 Hours

Max Marks:40

1. Using the substance B of mol. mass……determine the cryoscopic constant for the given solvent A and hence determine the mol. mass of the given solute C. Conduct a duplicate experiment. (35 Marks)

2. Determine the solid-liquid equilibrium for the binary system formed by the two substances A and B by the cooling curve method. Use the phase diagram to determine thecomposition of the given mixture C containing A and B (35 Marks)

3. Determine the concentrations of given Hydrochloric acid and Acetic acid solutions (A and B) by conductometric titration with sodium hydroxide.

4. Study the variation of miscibility temperature of phenol- water system by the addition of KCl and determine the concentration of the given KCl solution

5. Determination of coefficient of viscosity of glycerol-water system. Determine two unknown compositions from the graph

6. Construct the isothermal ternary phase diagram of the ternary liquid system A-B-C. Use the phase diagram to determine the composition by mass of the given mixture D of B and C.

7. a) By potentiometric titration, standardize the given HCl solution A with the given standard NaOH solution of normality …….
b) Determine the composition of the given mixture B of glycerol and water by refractometric method using at least 5 standard mixtures of the two components.

(35 Marks)

Record 5 Marks

KANNUR UNIVERSITY

M Sc IV Semester Examination March 20--

MSCHD03&04C15 Inorganic Chemistry Practical II

Time: 6 hours Max Marks: 40

1) Estimate the amount of chromium volumetrically and iron colorimetrically in the whole of the given solution of potassium dichromate and ferric alum. You are supplied with AR potassium dichromate and approximately 0.1N sodium thiosulphate solution and a standard solution containing……..g of ferric alum.

   Volumetry – 20 marks, Colorimetry -10 marks

2) Write in the first 10 minutes an outline of the method you would adopt for the estimation of…….. in a mixture of…….

   5 marks

For procedure writing any one of the following may be given

1) Ba gravimetric and Mg volumetric
2) Fe gravimetric and Ca volumetric
3) Ni gravimetric and Cu volumetric
4) Cu gravimetric and Zn volumetric
5) Fe colorimetric and Ca volumetric

Record…….. 5 marks.

KANNUR UNIVERSITY
MSc IV Semester Practical Examination March 20--
Time: 6 Hrs MSCHD03&04C17 Physical Chemistry Practical II Max. Marks. 40

1. Determine the rate constants for the hydrolysis of the given ester in presence of the given acids IA and IB at room temperature. Calculate at least 5 k values in each case. Also obtain the k values graphically.

2. Verify experimentally the Langmuir adsorption isotherm for the adsorption of oxalic acid on activated charcoal from aqueous solutions by using at least 5 standard solutions. Calculate the Langmuir parameters. Equilibrate 50 ml of the given solution of the acid with a known weight of charcoal and determine the concentration of the given acid using the isotherm.

(35 Marks)

Record 5 Marks

KANNUR UNIVERSITY

MSc IV Semester Practical Examination March 20--

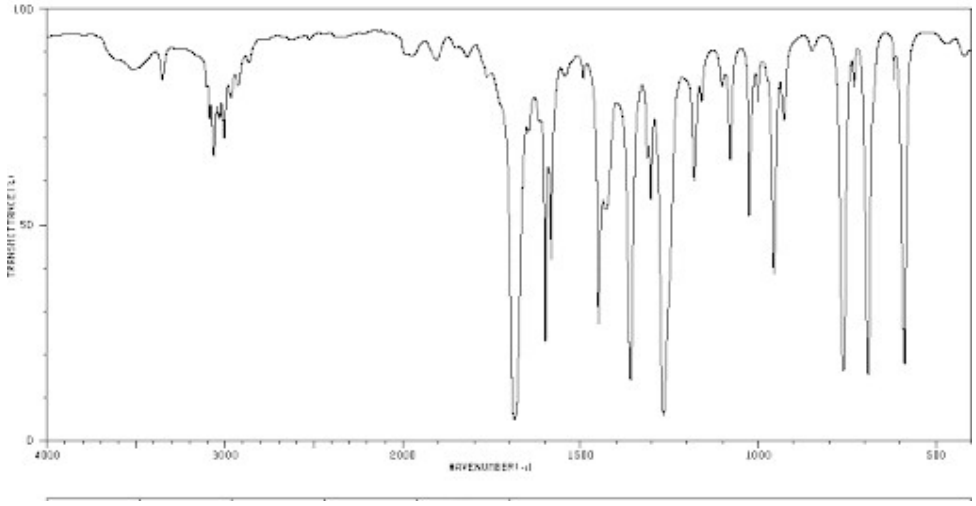
Time: 6 Hrs MSCHD03&04C16 Organic Chemistry Practical II Max. Marks. 40

1. Estimate the amount of phenol/aniline in the whole of the given solution. Marks:20

2. Convert the whole of the given acetanilide into p-nitro aniline. Exhibit the crude and the recrystallized samples of p-nitroacetanilide and p-nitro aniline for inspection. (After the first stage, the crude sample should be shown to the examiners before proceeding to the second stage) Marks:10

3. Analyze the given IR spectrum of ---------- and label the peaks a, b and c. Identify any two peaks Marks:5

   [Example given below: Acetophenone



   a) C=O peak
   b) Aromatic C-H peak
   c) Aliphatic C-H peak]

Record 5 Marks