

(Abstract)

MSc Chemistry Programme- Scheme , Syllabus and Pattern of Question papers (Ist and IInd semester only) under Choice Based Credit and Semester System (Outcome Based Education system- OBE) in Affiliated Colleges with effect from 2023 admissions - Implemented- Orders issued.

ACADEMIC C SECTION

ACAD/ACAD C4/16389/2023

Dated: 22.08.2023

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. U.O. No. Acad/C1/21246/2019 dated 09.08.2023
- 7. Minutes of the Meeting of the Adhoc committee for MSc Chemistry programme held on 10.08.2023
- 8. Syllabus submitted by the Convenor, Adhoc committee for MSc Chemistry Programme dated 18.08.2023

ORDER

- 1. A Curriculum Syllabus Monitoring Committee comprising the members of the Syndicate was constituted for the Syllabus revision of UG & 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 consideration of the Hon'ble Chancellor, considering the exigency of the matter, Ad hoc Committees were constituted vide paper read (3) above, & 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 Adhoc 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 paper read (5) above.
- 4. Revised Regulation for PG programmes under Choice Based Credit and Semester System (in OBE-Outcome Based Education System) was approved by the Vice Chancellor on 05.08.2023 and implemented w.e.f 2023 admission vide paper read (6) above.
- 5. Subsequently, as per the paper read (7) above, the Ad hoc committee for M.Sc Chemistry programme finalized the Scheme, Syllabus and Pattern of question papers of Ist & IInd semester M.Sc Chemistry programme to be implemented w.e.f 2023 admission
- 6. As per the paper read (8) above, the Convener, Ad hoc committee for M.Sc Chemistry submitted the finalized copy of the Scheme, Syllabus and Pattern of question papers of Ist & IInd semester M.Sc Chemistry programme for implementation w.e.f 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 of Ist & IInd semester M.Sc Chemistry programme under Choice Based Credit and Semester System (in OBE- Outcome Based Education System) in Affiliated

Colleges under the University w.e.f 2023 admission, subject to report to the Academic Council.

- 8. The Scheme, Syllabus and Pattern of question papers of Ist and IInd semester M.Sc Chemistry programme under Choice Based Credit and Semester System (in OBE- Outcome Based Education System) in Affiliated Colleges under the University w.e.f 2023 admission is uploaded in the University website
- 9. Orders are issued accordingly.

Sd/-Sajesh Kottambrath Assistant Registrar1 For REGISTRAR

To:

- 1. Principals of Affiliated Colleges offering MSc Chemistry Programme
- 2. Convener, Curriculum Syllabus Monitoring Committee.
- 3. Convener, Ad hoc Committee for M.Sc Chemistry 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) /All sections of Academic Branch/Computer Programmer
 - 4. SF / DF /FC

5. Web Manager (for uploading on the website)

Forwarded / By Order



(Abstract)

M.Sc. Chemistry Programme- Scheme (modified) , Syllabus and Model Question papers (III rd and IVth Semester only) under Choice Based Credit and Semester System (in Outcome Based Education system-OBE) in Affiliated Colleges -Implemented with effect from 2023 admissions - Orders issued

ACADEMIC C SECTION

ACAD/ACAD C4/16389/2023

Dated: 18.08.2024

Read:-1. U.O No. Acad C4/16389/2023 dtd 22.08.2023

- 2. Minutes of the meeting of BoS in Chemistry (PG) held on 22.05.2024
- 3. Modified Scheme & syllabus, submitted by the Chairperson, BoS in Chemistry (PG) vide e-mail dtd 13.06.2024
- 4. Minutes of the XXVIII th meeting of the Academic Council held on 25.06.2024

ORDER

- 1. As per the paper read (1) above, the Scheme, syllabus, Pattern of Question paper (I st and IInd Semesters only) of the M.Sc.Chemistry programme under Choice Based Credit and Semester System (in Outcome Based Education System- OBE) in Affiliated colleges were implemented w.e.f 2023 admission vide paper read (1) above.
- 2.Thereafter, the Meeting of the Board of Studies (BoS) in Chemistry, held on 22.05.2024 discussed & finalised the Syllabi of the IIIrd and IVth Semesters of the M.Sc.Chemistry programme under CBCSS in (Outcome Based Education System) to be implemented in affiliated colleges w.e.f 2023 admission, vide the paper read (2) above. The BoS recommended to change the IV th Semester scheme as per the approved Regulations. As per Clause 6.1 of the Regulations, the evaluation scheme for each Course shall contain two parts viz, a) Continuous Evaluation (CE) and End Semester Evaluation (ESE). 20% of weightage shall be given to the CE and 80% weightage shall be for the End Semester Examination. Therefore, the BoS modified the marks of MSCHE03 & 04 C18 to 20:5, instead of 30:5 and MSCHE04C20 Viva Voce to 40:10, instead of 40 as ESE and thereby corrected the total Marks distribution in IVth Semester as 360:90, instead of 370:80.
- 3. The Chairperson, BoS in Chemistry (PG) vide the paper read (3) above, submitted the Scheme (modified) and 3rd and 4th semester Syllabi and Model Question papers of the M.Sc.Chemistry programme in Affiliated colleges for implementing w.e.f 2023 admission.
- 4. The Vice Chancellor after considering the matter in detail, ordered to place the same before the Academic council for approval
- 5.The XXVIII th meeting of the Academic Council held on 25.06.2024, vide the paper read (4) above, considered the matter and approved the modified Scheme, IIIrd and IVth Semester syllabi and Model Question papers of the M.Sc.Chemistry Programme w.e.f 2023 admission under Choice Based Credit and Semester System (in OBE-Outcome Based Education System) in Affiliated colleges under the University in principle and accorded sanction to publish the same considering the urgency of the matter.
- 6. The Minutes of the Academic Council has been approved and published.
- 7.Therefore, the Scheme (modified), Syllabus and Model Question papers of the IIIrd and IVth Semesters of the M.Sc. Chemistry programme under Choice Based Credit and Semester System (in OBE-Outcome Based Education System) in Affiliated Colleges under the University w.e.f 2023 admission are uploaded in the University website.

Orders are issued accordingly.

Sd/-

ANIL CHANDRAN R
DEPUTY REGISTRAR (ACADEMIC)

For REGISTRAR

2. Convenor, Curriculum Syllabus Monitoring Committee

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) /All sections of Academic Branch/Computer Programmer

4. SF / DF /FC

5. Web manager (for uploading on the website)

6.EP V section



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KANNUR UNIVERSITY

SYLLABUS

For MSc Programme in CHEMISTRY in affiliated colleges-2023

Syllabus under Choice Based Credit and Semester System with effect from 2023 admission
OUTCOME-BASED EDUCATION - SYSTEM (OBE)

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1. PREFACE

The syllabi of the MSc programme in Chemistry 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

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

Master of Science in Chemistry is a Post Graduate level course that aims at an advanced level understanding of major concepts, theoretical principles, experimental aspects, and research aptitudes in chemical sciences. 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 Chemistry 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 Iaⁿ 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 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 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

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, and theoretical 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 in chemistry, including formulating 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 environmental science, materials science, pharmaceuticals, biochemistry, 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 on the basis of 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.

			_	-					
semest	Paper Code	Title	Hrs /wk	Exam Duratio n	Marks for ESA	Marks for CA	Total	Credit	
	MSCHE01C01	Theoretical Chemistry - I	4	3	60	15	75	4	
	MSCHE01C02	Inorganic Chemistry - I	4	3	60	15	75	4	
	MSCHE01C03	Organic Chemistry - I	4	3	60	15	75	4	
1	MSCHE01C04	Physical Chemistry - I	4	3	60	15	75	4	
	MSCHE01C05	Inorganic Chemistry Practical - I	3	Carried	over to s	semeste	r - II		
	MSCHE01C06	Organic Chemistry Practical - I	3	Carried	over to s	semeste	r - II		
	MSCHE01C06 Organic Chemistry Practical - I MSCHE01C07 Physical Chemistry Practical - I				over to s	semeste	r-II	15 3	
		Total :	25	0	240	60	300	16	
	MSCHE02C08	Theoretical Chemistry - II	4	3	60	15	75	4	
	MSCHE02C09	Inorganic Chemistry - II	4	3	60	15	75	4	
	MSCHE02C10	Organic Chemistry - II	4	3	60	15	75	4	
II	MSCHE02C11	Physical Chemistry - II	4	3	60	15	75	4	
	MSCHE01&02C05	Inorganic Chemistry Practical - I	3	6	40	10	50	2	
	MSCHE01&02C06	Organic Chemistry Practical - I	3	6	40	10	50	2	
	MSCHE01C&02C07	Physical Chemistry Practical - I	3	6	40	10	50	2	
		Total:	25		360	90	450	22	
T	MSCHE03001/02/03 Open Elective Paper I* (Multidisciplinary)		4	3	60	15	75	4	
			4	3	00		75	4	
	MSCHE03C12	Inorganic Chemistry III	4	3	60	15	75	4	
	MSCHE03C13	Organic Chemistry - III	4	3	60	15	75	4	
Ш	MSCHE03C14	Physical Chemistry - III	4	3	60	15	75	4	
	MSCHE03C15	Inorganic Chemistry Practical - II	3	Carried	Carried over to semester - IV				
	MSCHE03C16	Organic Chemistry Practical - II	3	Carried over to semester - IV					
	MSCHE03C17	Physical Chemistry Practical - II	3	Carried	over to s	semeste	r - IV		
	MSCHE03C18	Industrial Visit/Institutional Visit/Internship	2 2	Carried	over to s	semeste	r - IV		
		Total:	25		240	60	300	16	
	MSCHE04E01/02/03	Elective Paper II*	4	3	60	15	75	4	
	MSCHE04E04/05/06	Elective Paper III*	4	3	60	15	75	4	
	MSCHE03&04C15	Inorganic Chemistry Practical - II	3	6	40	10	50	2	
IV	MSCHE03&04C16	Organic Chemistry Practical - II	3	6	40	10	50	2	
	MSCHE03&04C17	Physical Chemistry Practical - II	3	6	40	10	50	2	
	MSCHE03&04C18	Industrial Visit/Institutional Visit/Internship			20	5	25	2	
	MSCHE04C19	Project (With Presentation)	8		60	15	75	6	
	MSCHE04C20	Viva Voce (General)		12	40	10	50	4	
	~	25		360	90	450	26		

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

Semesterwise Split-up of Marks

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

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

	ELECTIVE PAPERS									
Sem	Elective No	Paper Code	Title							
		MSCHE03O01	Food Chemistry							
ш	I (Open Elective/	MSCHE03O02	Environmental Chemistry and							
	Multidisciplinary	Wiscing of 5	Disaster Management							
		MSCHE03O03	Medicinal Chemistry							
	II	MSCHE04E01	Interdisciplinary topics and							
IV			instrumentation techniques							
		MSCHE04E02	Computational Chemistry							
		MSCHE04E03	Biochemistry							
		MSCHE04E04	Nanomaterial Chemistry							
IV	III	MSCHE04E05	Polymer Chemistry							
		MSCHE04E06	Material Chemistry							

6.4 Project Work and Viva Voce

a) Each student shall carry out project work in one of the broad areas of theoretical/Organic/physical/environmental/inorganic 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

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				

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

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 I^{ts} 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/Presenta tion 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								
SI N o	% of Marks	Grade	Interpretation	Range of Grade Points	Class				
1	90 and above	A+	Outstanding	9.0 - 10	First class with				
2	80 to below 9	Α	Excellent	8.0 - 8.9	distinction				
3	70 to below 8	В	Very Good	7.0 - 7.9	First class				
4	60 to below 7	С	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. Bonafide certificate shall be in the following format

	CERTIF	TCATE
Kannur University i	n partial fulfilment of the requi .(subject), is a Bonafide record	rements of Post Graduate Degree in of studies and work carried out by under my supervision and guidance.
Office seal Date	Signature, name, des	ignation, and official address of the Supervisor.
6.8.4. Declaration	by the student shall be in the	following format:
	DECLARATION	
		date) hereby declare that this project titled fide record of studies and work carried out by me
under the supervision address of the sup	on ofervisor), and that no part of	this project, except the materials gathered from a ward of any degree or diploma, or other similar
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	
А	5 out of 6 questions (short answer questions)	5 x 8 min = 40 min		5	×	3	=	15	25	1,2 (Remember, Understand)
В	3 out of 5 questions (paragraph questions)	3 x 20 min = 60 min	3	3	×	6	=	18	30	5, 6 (Evaluate, Create)
С	3 out of 5 questions (essay-type questions)	3 x 25 min = 75 min	3	3	×	9	=	27	45	3, 4 (Apply, Analyze)
					Т	ota	ıl =	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-1			
MSCHE01C01: THEORETICAL CHEMISTRY - I			
t: 4		TIME: 72 HOURS	

18 Hours

18 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

QUANTUM MECHANICS-I

CO 5. Apply HMO theory to simple conjugated systems

Course Content

UNIT -1

UNIT - II

Credit: 4

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 Schrödinger 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.

QUANTUM MECHANICS - II

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 - α r2 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 H₂+ ion – valence bond treatment of the ground state of hydrogen molecule – MO treatment of homonuclear diatomic molecules (quantitative) – Li₂, Be₂, N₂, O₂, O₂+, O₂-, F₂ 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

REFERENCES

Hill

Hill

- 1. N Levine, Quantum Chemistry 5th Ed. Prentice Hall India
- 2. R. Anantharaman, Fundamentals of Quantum Chemistry, Mc Millan India
- 3. A. K. Chandra, Introductory Quantum Chemistry 4th Ed. Tata Mc Graw
 - 4. D. A. McQuarrie Quantum Chemistry, University Science Books
- 5. L. Pauling and W.B Wilson, Introduction to Quantum Mechanics, McGraw
 - 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

MSCHE01C02: 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	18 Hours
	SOLVENTS	

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 non-aqueous solvents like HF, N_2O_4 , and SO_2 – chemistry of molten salts as non-aqueous solvent systems – solvent properties – room temperature molten salts – non reactivity 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, Neutron Activation Analysis, Tracer techniques, Medicine, Industry

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

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 dicarbaclosododecaboranes ($C_2B_{10}H_{12}$ - 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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- 2. Vogel's Textbook of Quantitative Chemical Analysis Fifth Edition
- 3. Bodie Douglas, Darl H Mc Daniel AND John J Alexander, Concepts and models of Inorganic Chemistry, John Wiley and Sons Inc 3rd edition
- 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
- H J Arniker, Essentials of Nuclear Chemistry, New Age International, New Delhi 4th edition 1995
- 10. J D Lee, Concise Inorganic Chemistry (IVth edition) Oxford University Press
- 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

MSCHE01C03: 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	18 Hours
	REARRANGEMENTS	
C4		1_41 41_41_

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	18 Hours
	REACTIONS			

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	18 Hours
	REACTIONS			

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:

- 1. R. Bruckner, Advanced Organic Chemistry: Reaction Mechanism, Academic Press, 2002.
- 2. F.A. Carey, R.A. Sundberg, Advanced Organic Chemistry, Part B: Reactions and Synthesis, 5/e., Springer, 2007.
- 3. J. Clayden, N. Greeves, S. Warren, P. Wothers, Organic Chemistry, Oxford University Press, 2004.
- 4. R.O.C.Norman & J.M.Coxon, Principles of Organic Synthesis, 3/e, Nelson Thornes
- 5. J. March, M.B. Smith, March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 6/e, Wiley, 2007.
- 6. Ahluwalia Mukherjee and Singh, Organic reaction mechanisms
- 7. Maya Shankar Singh, Advanced organic chemistry: reactions and mechanisms, Pearson
- 8. Peter Sykes, A guidebook to mechanism in organic chemistry, 6th Ed Pearson
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- 10. P.S. Kalsi, Organic reactions & their mechanisms, 3/e revised, New Age International Publishers.
- 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.

MSCHE01C04: 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	18 Hours
	EQUILIBRIA			

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.

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	18 Hours
	CORROSION	

Energy storage devices: Batteries- Working of Lithium-ion battery. Basics of supercapacitors, Classification with examples. Electrostatic double layer capacitors (EDLC) and Psuedo capacitorsworking 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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- 2. S. Glasstone-"Thermodynamics for chemists"—Affiliated East West publication.
- 3. Lewis and Randal-"Thermodynamics"-McGraw-Hill.
- 4. Daniels and Alberty-"Physical Chemistry"- John Wiley.
- 5. "Mathematics of physics and chemistry"- Murphy, George M., Margenau, Henry
- 6. S. Glasstone-"Theoretical electrochemistry"-East-West Books
- 7. L.I.Anthropov-"Theoretical electrochemistry"-Mir publishers.
- 8. Bockris and Reddy-"Modern electrochemistry"-Springer
- 9. G.W. Castellan "Physical chemistry"- Narosa
- 10. I. Pregogine-"Introduction of Irreversible to thermodynamics process"-Interscience
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- 14. Fontana and Greene Corrosion Engineering:
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- 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

MSCHE02C08: 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,	18 Hours
	MATRICES			

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 – Γ cart, Representation generated by Cartesian coordinates positioned on the atoms of a molecule (H_2O and SO_2 as examples) - Γ regular – reducible and irreducible representations – construction of irreducible representation by reduction.

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

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 – BF₃ CH₄, PCI₅ as examples- Application to MO theory-. Group orbitals and their construction-Projection Operator method and pictorial method- Transition Moment Integral. Examples H₂O, NH₃, 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 H₂O, NH₃, CH₄, BF₃, N₂F₂

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. H₂O, N₂O and CO₂ molecules)

UNIT –IV	SPECTROSCOPY II	18 Hours
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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.

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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,
- 6. Manas Chanda "Atomic Structure and Chemicals Bonding including Molecular Spectroscopy, 4th Edn," Tata McGraw Hill
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- 9. S Swarna Lakshmi, T Saroja, and R M Ezhilarasi "A Simple Approach to Group Theory in Chemistry" Universities Press
- 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

MSCHE02C09: 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 dⁿ ion. selection rules for d-d transitions – effect of spin-orbit coupling and vibronic coupling on electronic transitions - Orgel diagram of transition metal complexes(d¹ to d⁹ 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	18 Hours
	CHEMISTRY	

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
- 2. J C Bailer, Chemistry of coordination compounds, Reinhold
- 3. F Basolo R Johnson, Coordination Chemistry, Benjamin Inc
- 4. D Banergea, Coordination Chemistry, Tata McGraw Hill
- 5. D N Sathyanarayana, Electronic Absorption spectroscopy, and related techniques, Universities Press
- 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
- 9. R L Dutta and A Syamal, Elements of magneto chemistry, S Chand and Company Ltd
- 10. Glen E Rodgers, Inorganic and solid state chemistry, Cengage Learning
- **11.** R.S.Drago, Physical Methods in Chemistry, W.B.Saunders Company, Philadelphia, London, 1976.

MSCHE02C10: 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	18 Hours
	ASYMMETRIC SYNTHESIS		

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. HIO₄, OsO₄, and mCPBA and their applications. Synthetic applications of the following reagents – Gillman's reagent, LDA, 1, 3 dithianes, DDQ, DDC, SeO₂, Bakers yeast, NBS, Wilkinsons's catalyst. Asymmetric reductions using BINAL-H. Asymmetric hydroboration using IPC2BH and IPCBH2. Reduction with CBH reagent.

- 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

MSCHE02C11: 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	18 Hours
	AND QUANTUM STATISTICS		

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	18 Hours	

CRYSTALLOGRAPHY

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 TiO₂(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- paramagnetic- 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.

- 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
- 9. UriShmueli. "Theories and techniques of crystal structure determination" Oxford University Press,

10.2007.

- 10. Christopher Hammond. "The basics of crystallography and diffraction" Third edition, 2009, Oxford University Press.
- 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

MSCHE01&02C05: INORGANIC CHEMISTRY PRACTICAL—I (1st and 2nd semester)

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:

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.

MSCHE01&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

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) Preparation of polymer compounds (minimum 2 compounds):

PMMA, Polystyrene, Polyesters, PANI (Exhibit during examinations)

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.

MSCHE01&02C07: PHYSICAL CHEMISTRY PRACTICAL - I

(I st and 2 nd 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-BaSO₄)

Conductance titrations. HCl vs NaOH, (HCl+ HOAc) vs NaOH, AgNO₃ 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 + HgI₂ → K₂HgI₄ 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)

- 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 Williard, 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

SEMESTER III MSCHE03C12 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	18 Hours
	AND RELATED			

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, Fe₂(CO)₉, Co₂(CO)₈, Mn₂(CO)₁₀, Tc₂(CO)₁₀, Re₂(CO)₁₀, Metal-metal bonding – Rhenium complexes , Carbonyl clusters (low nuclearity carbonyl clusters (LNCC) – Os₃CO₁₂, Ir₄CO₁₂ and high nuclearity carbonyl clusters (HNCC) – Rh₆CO₁₆, 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	18 Hours
	BLOCK ELEMENTS	

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 & illminite

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 O₂ 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

- 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.

MSCHE03C13: 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: Illucidate and analyse the structure of different heterocyclic compounds and biomolecules

Course Content

UNIT I	ELECTRONIC AND IR SPECTROSCOPY	18 Hours
Colour and light absor	rption – the chromophore concepts – theory of elect	ronic 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 λ max 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 18 Hours CHEMISTRY

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, Modeern 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 organioc chemistry part 1 and 11, New central book

	SEMESTER – III
MSCF	IE03C14 : PHYSICAL CHEMISTRY – III

Credit 4 Time: 72 Hours

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

- C.O.1. To get an understanding of kinetic aspect of chemical reactions.
- C. O.2. To infer kinetic approach of Catalysis.
- C.O.3. To get a knowledge on surface chemistry and different surface catalysed reactions.
- C.O.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 H₂-CI₂ and H₂-Br₂-decomposition of acetaldehyde-Rice Herzfeld mechanism- Branching chain-H₂O₂ 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 & Taft equation.

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-Langmuir - Hinshelwood -The Eley-Ridel mechanism -flash desorption. Superhydrophobic 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 effecting 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 effecting 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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- 2. S.Glasstone, K.J. Laidlerand Eyring-"The Theory of rate processes"-McGraw Hils
- 3. J. Rajaram and J.C. Kuriakose- "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 MSCHE03O01: 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	18 Hours
	AND FLAVOR ENHANCERS	

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,	18 Hours
	PRESERVATIV	ES, A	ND CONT	AMINATION	

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 AND	18 Hours
	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	18 Hours
	NANOTECHNOLO	OGY IN FOOD		

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.

- 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 MSCHE03002: ENVIRONMENTAL CHEMISTRY AND DISASTER MANAGEMENT

Credits 4	Time: 72 Hours

Course outcome: 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	18 Hours
UNII – I	POLLUTION			

Components of environment. Factors effecting 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 SO₂, NO_X, CO, H₂S, 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,	18 Hours		
	POLLUTION	AND	INSTRUMENTAL	
	METHODS IN O			

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	18 Hours
	DISASTER MANAGEMENT	

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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- Prakashan Mandir, Meerut
- 2. B K Sharma and H Kaur, Water pollution, Krishna Prakashan Mandir, Meerut
- 3. T H Y Tebbutt, Principles of water quality control A, Butterworth-Heinemann
- 4. Anil K De, Environmental chemistry 4th edn. New age International Pvt Ltd
- 5. Cleaning our environment-A chemical perspective 2nd dent, American Chemical Society
- 6. S K Banerjee, Environmental chemistry, Goel Publishing house, Meerut
- 7. L W Moore and E A Moore, Environmental chemistry, McGraw Hill Publication, Newyork
- 8. Gary W Vanloon and Stephen J Duffy, Environmental chemistry-A global perspective,Oxford University Press
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- 10. Alexander, D. Natural Disasters, ULC press Ltd, London, 1993
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- 12. Chakrabarty, U. K. *Industrial Disaster Management and Emergency Response*, AsianBooks Pvt. Ltd., New Delhi 2007.
- 13. Abarquez I. & Murshed Z. Community Based Disaster Risk Management: FieldPractitioner's Handbook, ADPC, Bangkok, 2004.
- 14. Goudie, A. Geomorphological Techniques, Unwin Hyman, London 1990.
- 15. Goswami, S. C. *Remote Sensing Application in North East India*, Purbanchal Prakesh, Guwahati, 1997.
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- 17. Disaster Management in India, Ministry of Home Affairs, Government of India, NewDelhi, 2011.
- 18. National Policy on Disaster Management, NDMA, New Delhi, 2009.
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- 21. Coppola P Damon, 2007. Introduction to International Disaster Management,
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- Anu Kapur, Vulnerable India- A Geographical Study of Disasters, Sage Publications India
- 24. V K Ahluwalia, Environmental Pollution and Health, TERI Press
- 25. B K Sharma and H Kaur, Thermal and Radioactive Pollution, Krishna's Educational Publishers
- 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
- 32. NFPA Codes and Standards
- 33. Central Motor Vehicle Rules India- 1989, Chapter 5
- 34. K. Palanivel, J. Saravanavel, S. Gunasekaran, Disaster management, 1 st Edn., Allied Publishers New Delhi, 2015.
- 35. S. Modh, Managing Natural Disasters, Mac Millan publishers India LTD., 2010.
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MSCHE03003: 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, and misuse of drugs

Course Content

UNIT-I	DRUGS:	CLASSIFICATION,	18 Hours
	MECHANISM, AN		

Introduction: Nature and source of drugs – important terminologies in pharmaceutical chemistry. Classification and nomenclature of drugs: biological and chemical classification, classification of drugs according to commercial considerate, classification by lay public, nomenclature of drugs, some important heterocyclic drug systems and their applications.

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. Synthesis of medicinal compounds like Aspirin, Paracetamol and Chloramine-T. Brief study on Anticancer drugs and drugs acting on kidney and AIDS treatment.

UNIT-II ANTIBACTERIAL, ANTIBIOTICS, ANTISEPTICS, AND DISINFECTANTS

Antibacterial drugs: Sulpha drugs; sulphanilamides – properties of sulphanilamides, mechanism of action of sulfa drugs, sulphadiazine, sulphapyridine, cibazole, sulphafurazole, Prontosil – Antibiotics; classification of antibiotics, chloramphenicol, penicillin, streptomycin, tetracycline, macrolides. Antiseptic and disinfectants: Phenols and its derivatives – halogen compounds –dyes – organic mercurials – formaldehyde and its derivatives – nitrofuran derivatives – cationic surface active agents. Anti biotics- Discovery and its importance. Examples of antibiotics –Antibiotic misuse .Anti histamines- examples , anti-malarial, antipyretics, Diuretics and anti-ulcer drugs. Drugs acting on Central Nervous System, Drugs acting on Peripheral Nervous System. Cardiovascular drugs classification and examples.

UNIT – III ANESTHETICS, ANALGESICS, AND ANTI- 18 Hours INFLAMMATORY AGENTS

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

Analgesics: Introduction. Narcotic analgesics – natural narcotic analgesics; morphine, heroin, apomorphine – synthetic narcotic analgesics; pethidine, morphinan, benzomorphan – non narcotic analgesics; salicylic acid derivatives, the paraminophenol, the pyrazole, indolyl and aryl acetic acid derivatives. Anti-inflammatory agents. NSAIDs and their derivatives. A brief explanation of their mode of action. Steroids-Classification and its effects.

UNIT-IV DRUGS EFFECTS, DESIGN, AND MISUSE 18 Hours

Classification of drugs of abuse –Narcotics, CNS Stimulants examples and effects, Depressants, Hallucinogens examples and effects, Sedatives, hypnotics, example and effects, Cocaine, Opioids, Cannabis and Inhalants examples and effects. Tranquilizers. Drug dependence, withdrawal symptoms, tolerance and addiction. Synthetic drugs, Amphetamine and substituted amphetamine-MDMA, structure and its adverse effects. Lysergic acid diethylamide structure and its adverse effects. In-silico and computer aided drug design. Introduction to computer aided drug design (CADD). Drug likeliness and Pharmaco kinetics- A brief explanation - Pharmaco dynamics- Modes of drug action, Docking studies- Protein-Ligand docking techniques, Dose response relationship - Lethal Dose, EC 50 or ED 50 Therapeutic index.

REFERENCES

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- 2. K D Tripathi, Essentials of medical pharmacology, 6th edn, 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 Yog Eeswari, 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 II* MSCHE04E01: INTER DISCIPLINARY TOPICS AND INSTRUMENTATION **TECHNIQUES** Credits: 4 Time: 72 Hours Course outcome: 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; diagnosing, 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 Fe²⁺ and Fe³⁺

- 1. V K Alhuvalia, Green Chemistry, Ane books
- 2. P T Anastas and J C Warner Green Chemistry Oxford
- 3. G A Ozin, A C Arsenault, Nano chemistry RSC
- 4. Diwan, Bharadwaj, Nano composites, Pentagon
- 5. V S Muralidharan, A Subramania, Nano science and technology, Ane books
- 6. Willard Merit, Dean, Kettle, Instrumental methods of analysis, 7th ed CBS.

7. Chatwal- Anand, Instrumental analysis of chemical analysis, Himalaya publishing house

MSCHE04E02: COMPUTATIONAL CHEMISTRY

Credits: 4 Time: 72 Hours

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

- C 01: Understand the theoretical foundations of computational chemistry. Analyze the importance of quantum mechanics in understanding molecular behavior.
- C02: Classify and evaluate computational methods in chemistry. Categorize computational methods based on their approaches and applications.
- C03: Apply *ab Initio* and semi-empirical methods in computational chemistry. Assess the strengths and limitations of these methods.
- C04: Demonstrate proficiency in the use of basis sets and molecular orbitals in computational chemistry.
 - (i) Discuss the role of basis sets in electronic structure calculations.
 - (ii) Critically evaluate the advantages and limitations of different basis sets.
- C05: Utilize Density Functional Theory (DFT) to study molecular systems.
 - (i) Understand the foundations of DFT and its significance.
 - (ii) Apply various DFT functionals for electronic structure calculations.
- C06: Employ molecular dynamics simulations to study molecular structures and interactions.
 - (i) Explain the principles of molecular dynamics.
 - (ii) Implement force fields for molecular simulations.
 - (iii) Analyze molecular dynamics trajectories to understand structural changes and interactions.
- C07: Conduct computational spectroscopy to predict vibrational, electronic, and NMR spectra. Prepare input programs in Gaussian / GAMESS format for various calculations.

Course Content

UNIT – I COMPUTATIONAL CHEMISTRY – I 18 Hours

Basic aspects (8 Hrs): Theoretical foundations of computational chemistry – Historical development and role in modern chemistry – Theory, computation & modeling – Definition of terms – Need of approximate methods in quantum mechanics – Computable quantities – Structure, potential energy surfaces and chemical properties – Cost and Efficiency – Classification of computational methods.

Hartree – Fock Method (10 Hrs): *Ab initio* methods: Hartree – Fock method, Self Consistent Field (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 and electron correlation – Introduction to post-HF methods.

UNIT – II COMPUTATIONAL CHEMISTRY – II 18 Hours

Semiempirical methods (8 Hrs): the basic principle of SCF-SE methods – Neglect of diatomic differential overlap approximation (NDDO) – intermediate Neglect of differential overlap

approximation (INDO) – complete Neglect of differential overlap approximation(CNDO) – parameterization – modified intermediate Neglect of differential overlap (MINDO) – modified NDDO and MNDO models – Austin model 1(AM1).

Density Functional Theory (DFT) (10 Hrs): Introduction – Representability problems – Hohenberg-Kohn theorems – Kohn-Sham theory – reduced density matrix methods – local density approximation application – generalized gradient approximation, hybrid functionals – performance and properties of density functional methods. Comparison between DFT and HF.

UNIT -III | COMPUTATIONAL CHEMISTRY - III | 18 Hours

Basis sets (9 Hrs): Hydrogen-like, Slater-type & Gaussian type basis functions, classification of basis sets – minimal, double zeta, triple zeta, split-valence, polarization and diffuse basis sets – contracted basis sets, Pople-style basis sets: Nomenclature, calculation of number of basis functions and primitives used in a given basis set – correlation consistent basis sets, basis set superposition errors (BSSE), effect of choice on method / basis set (model chemistries) on CPU time

Molecular Mechanics (9 Hrs): Basic principles – developing force field – the stretch energy – the bending energy – torsional energy – the Van der Waals energy – the electrostatic energy – cross terms – parameterizing the force field – geometries and frequencies calculated by MM – strength and weakness of MM – Force fields in molecular docking.

UNIT – IV COMPUTATIONAL CHEMISTRY – IV 18 Hours

Molecular Dynamics (MD) (8 Hrs): Basic principles – Calculation of simple thermodynamic properties – energy, heat capacity, pressure and temperature, phase space, periodic boundary conditions, monitoring the equilibration, analyzing the results of a simulation, error estimation – MD using simple models – continuous potentials, finite difference methods, choosing the time step

Applications (10 Hrs): Prediction of molecular properties using computational chemistry – Equilibrium molecular geometry – Applications in vibrational spectroscopy: calculating IR and Raman frequencies of molecules – Applications in UV and NMR spectroscopy – Applications in chemical thermodynamics

Understanding molecular geometry input (Z-matrix input) – Writing Z-matrix input of simple molecules with $N_{atom} < 12$ – Preparing computational chemistry input program in Gaussian / GAMESS format to calculate various molecular properties such as single point energy, geometry optimization, frequency calculation etc.

- 1. Leach AR. *Molecular Modelling : Principles and Applications*. 2nd ed. Harlow England: Prentice Hall.
- 2. Cramer CJ. Essentials of Computational Chemistry: Theories and Models. 3rd ed. Somerset: Wiley;.

- 3. Frank Jensen, *Introduction to Computational Chemistry*, John Wiley & Sons ltd.
- 4. David Young, Computational Chemistry- A Practical Guide for Applying Techniques to Real World Problems, Wiley -Interscience
- 5. Tamás Veszprémi and Miklós Fehér, *Quantum Chemistry: Fundamental and applications*, Springer-India
- 6. Errol G. Lewars, Computational Chemistry: Introduction to the theory and applications of molecular quantum mechanics, 2nd edn., Springer
- 7. I.N. Levine, *Quantum Chemistry*, 6th Edition, Pearson Education Inc..
- 8. Szabo A Ostlund NS. *Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory.* Mineola NY: Dover Publications.
- 9. W. Koch, M.C. Holthausen, *A Chemist's Guide to Density Functional Theory*, Wiley-VCH Verlag.
- 10. David B Cook, Handbook of computational quantum chemistry, Oxford University Press

MSCHE04E03: BIOCHEMISTRY

Credits 4 TIME: 72 Hours

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

- CO 1: To impart advanced knowledge about biomolecules as building blocks of life
- CO 2: To discuss the metabolisms of carbohydrates, lipids, proteins and nucleic acids in organisms
- CO 3: To discuss the significances of endocrine glands and their hormones in human body
- CO 4: To apply the knowledge of endocrine hormonal action in understanding endocrine disorders
- CO5: To understand the importance of enzymes in metabolic reactions

Course Content

UNIT: I INTRODUCTION TO BIOCHEMISTRY 18 Hours

Biomolecules - Carbohydrates - monosaccharides -ring structure of sugars - formation of disaccharides- reducing and non reducing disaccharides - polysaccharides- homo and hetero polysaccharides - structural and storage polysaccharides - biological function of carbohydrates. Lipids - building blocks of lipids - fatty acids, classification - essential and non-essential fatty acids- lipids in membranes- glycerophospholipids, galactolipids, sulpholipids, sphingolipids, sterols. Amino acids, Classification - Essential and non-essential

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

UNIT: II ENZYMES 18 Hours

Enzymes - Classification, Mechanism of enzymatic reactions, kinetics of enzymatic reactions, Michaelis Menton model, Measurement of significance of KAMAX and Vmax perfect enzymes. Inhibition of enzymatic reactions. Kinetics of competitive and non-competitive Inhibition. Allosteric enzymes Mechanism of enzymatic catalysis by Lysozyme and carboxypeptidase, 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. Clinical uses of enzyme therapy, Enzymes and recombinant DNA technology. Genomic Library.

Unit: III NUCLEIC ACIDS AND HORMONES 18 Hours

Nucleic acids: Nucleic acid bases, Nucleosides, nucleotides, structure of DNA, RNA and its classifications, 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 - Name and functions in body, Anti-hormones. Endocrine disorders: Gigantism, Acromegaly, dwarfs, pigmies, Diabetes insipidus

Unit IV	BIOLOGICAL	OXIDATION	AND	18 Hours
	METABOLISM			

Carbohydrate metabolism-Carbohydrate the source of energy, Biosynthesis of lactose, sucrose and starch; 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: Fatty acid oxidation - Franz Knoop's experiment; β oxidation of saturated, unsaturated and odd carbon fatty acids;; Biosynthesis of saturated fatty acids; Elongation and desaturation of fatty acids; Regulation of fatty acid metabolism; Cholesterol biosynthesis and its regulation; Prostaglandins- classification, structure and biosynthesis and biological role Protein and amino acid metabolism:. Over view of the fate of carbon skeletons of amino acids, Gamma-Glutamyl cycle, Degradation of amino acids, oxidative and nonoxidative deamination, transamination, decarboxylation, detoxication of ammonia - Urea cycle, catabolism of carbon skeletons of amino acids - ketogenic and glucogenic amino acids.

- 1. Nelson, D.L. and Cox, M.M.(2005). Lehninger Principles of Biochemistry, W.H. Freeman & Com
- 2. Widmaier, E.P.,Raff, H. and Strang, K.T.(2008). Vander, Sherman, Luciano's Human Physiology, McGraw-Hill Higher Education.
- 3. The text book of biochemistry (for medical students) DM Vasudevan, Sreekumari S, JAYPEE Brothers NEW DELHI.
- 4. Fundamentals of Biochemistry by J. L. Jain, Sunjay Jain and Nitin Jain (2008) Publishers: S. Chand & Co Ltd
- 5. Darnell, J., Lodish, H. and Baltimore, D.(2008). Molecular Cell Biology, Scientific American Books. Paper 18-BCHP
- 6. Voet, D and Voet, J.G, (2009) Biochemistry, John Wiley and Sons, N.Y. USA.
- 7. Garret, R.H. and Grisham, C.M. (2005) Biochemistry 3rd edition, Thomson Learning INC.
- 8. Lehninger: Principles of Biochemistry (2013) 6th ed., Nelson, D.L. and Cox, M.M., W.H. Freeman and Company (New York).
- 9. Textbook of Biochemistry with Clinical Correlations (2011) 7th ed., Devlin, -T.M., John Wiley & Sons, Inc. (New York).
- 10. Biochemistry (2012) 7th ed., Berg, J.M., Tymoczko, J.L. and Stryer L., W.H. Freeman and Company (New York).
- 11. Harper□s Biochemistry (2012) 29th ed., Murray, R.K., Granner, D.K., Mayes and American Books. Paper 18-BCHP
- 12. Principles of Biochemistry Geoffrey L Zubey, William W parson Pennis E Vance, WMC Brown publishers.
- 13. Biochemistry: Lubert Stryer. and Hall, J.E., Library of congress cataloguing-in publication Data, Bery, Jeremy mark ISBN.

ELECTIVE PAPER III* MSCHE04E04: NANOMATERIAL CHEMISTRY

Credits: 4 Time: 72 Hours

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

CO1: Understand the history and mile stones in nanotechnology.

CO2 :To Provide an insights to various physical and chemical synthesis methods of nanomaterials

CO3:To apply the basic knowledge of spectroscopy techniques in nano material characterization CO4:Analyse the applications of nanomaterials in energy, environment, electronic and magnetic fields.

Course Content

UNIT I INTRODUCTION TO NANO SCIENCE 18 Hours

History of Nanotechnology, Feynman's vision on Nano Science & technology, bulk vs nanomaterials. nanoscale architecture. Classification based on the dimensionality, Zero-dimensional nanostructures: metal, semiconductor and oxide nanoparticles. One-dimensional nanostructures: nanowires and nanorods, Two-dimensional nanostructures: Thin films, Three-dimensional nanomaterials, Special Nanomaterials: Carbon fullerenes and carbon nanotubes, Size and shape dependent properties, Melting points and lattice constants, Surface Tension, Mechanical properties, Optical properties: Surface plasmon resonance in metal nanoparticles and quantum size effect in in Semiconductors. Recent developments, challenges and future prospects of nanomaterials.

UNIT II DESIGN AND SYNTHESIS OF 18 Hours NANOMATERIALS

Physical Methods for synthesis of nanomaterials: Physical Vapour deposition, chemical vapour deposition method and Electrospinning, arc discharge, RF plasma, ion sputtering, laser ablation, Microwave irradiation Gamma radiation.

Chemical Methods for synthesis: co-precipitation, hydrothermal and solvothermal synthesis, electrochemical synthesis, sol-gel synthesis, self-assembly, self-assembled monolayers, directed assembly, layer-by-layer assembly. Lithographic Techniques: photolithography, other optical lithography (EUV, X-ray, LIL), Particle-beam lithography (e-beam, FIB, shadow mask evaporation), probe lithography.

UNIT III	CHARACTERISATION TECHNIQUES	18 Hours
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X-ray Spectroscopy techniques: powder XRD, X-ray fluorescence spectroscopy, X-ray photoelectron

spectroscopy, UV-visible spectroscopy, FT-IR spectroscopy, Raman spectroscopy, absorption and emission Spectroscopy. Microscopy Techniques: Optical microscopy, fluorescence and confocal microscopy, Ellipsometry. Electron microcopies TEM, SEM, SIMS, Probe techniques; Scanning tunneling microscopy (STM), atomic force microscopy (AFM), scanning near field optical microscopy (SNOM), scanning ion conducting microscopy (SICM)., Dynamic light scattering (DLS), Contact angles.

UNIT IV APPLICATION OF NANOMATERIALS 18 Hours

Nanomaterials for Energy and Environment: sustainable energy production based on renewable energy sources: solar cells, dye sensitized solar cell, Hydrogen energy, hydrogen production by water splitting, hydrogen storage. Fuel cells, Types of fuel cells. Batteries, Li-ion battery, Na-ion battery, General properties of electrochemical capacitors, Supercapacitor, Electrical double layer capacitor, pseudocapacitor. Nanomaterials for environmental Remediation, Photocatalysis, Water purification using nanomaterials, desalination of water, Solid waste removal, Porous materials to store clear energy gases, Metal organic frame works(MOFs). Nanoelectronic and nanomagnetic Devices. Nanoscale photonic devices including photonic band gap materials.

- 1. Introduction to Nano Science and Nanotechnology, by K Chattopadhyay, PHI Learning Pvt. Ltd. New Delhi 2019, ISBN-13: 978-81-203-3608-7.
- 2. Characterization of Materials Vol 1 &2, by Elton N. Kaufmann, John Wiley and Sons Publication, 2003. New Jersey.
- 3. Principles of instrumental analysis, Douglas A Skoog, Donald M West, Saunders College, Philadelphia. Publisher: Cengage; 6 edition (1 November 2014) ISBN-13: 978-81-315- 25579.
- 4. NANO: The Essentials- Understanding Nano Science and Nanotechnology, by T Pradeep, Tata McGraw Hill Education Pvt. Ltd. New Delhi) ISBN-13: 978-0-07- 061788-9
- 5. Geoffrey A Ozin and Andr C Arsenault, Nanochemistry: A Chemical approach to nanomaterials, The Royal Society of Chemistry, 2005
- 6. Nanostructures and Nanomaterials- Synthesis, Properties & applications by Guozhong Cao, Imperial college Press, (2006). Publisher: World Scientific Publishing Company; 2 edition (4 January 2011) ISBN-13: 978-9814324557
- 7. Jingbio louise Liu, Sajid Bashir, Advanced Nanomaterials and their applications in Renewable energy, Elsevier, 2015.
- 8. Tetsuo Soga, Nanostructured Materials for Solar Energy Conversion, Elsevier, 2006.

9. G.A. Nazri and G. Pistoia, Lithium Batteries: Science and Technology, Kluwer Academic Publishers, Dordrecht, Netherlands, 2004.

MSCHE04E05- POLYMER CHEMISTRY

Credits: 4 Time: 72 Hours

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

CO1: To get an understanding about properties of polymers and mechanism of different types of polymerization.

CO2: To get a knowledge on different characterization in polymers.

CO3: To identify different polymerization process and polymer reactions

CO4: To differentiate applications of different polymers

Course Content

UNIT – I	INTRODUCTION TO		POLYMER	18 Hours
	CHEMISTRY			

Classification of polymers – natural and synthetic polymers – nomenclature of polymers – mechanism and kinetics of step reaction polymerization – gelation – gel point – experimental observation of gel point – radical chain polymerization and its mechanism and kinetics – effect of temperature and pressure on chain polymerization – living polymers – coordination polymerization – Ziegler Natta catalyst – polymerization of nonpolar alkene monomers – ring opening polymerization – mechanism of copolymerization. Molecular forces and chemical bonding in polymers – intermolecular forces and physical properties – configuration of polymer chains, mechanical properties of crystalline polymers – crystalline melting point – glassy state and glass transition – factors influencing the glass transition temperature – glass transition temperature and its effects on properties of polymers

UNIT – II CHARACTERIZATION OF POLYMERS 18 Hours

Criteria of polymer solubility – effect of molecular mass and solubility – solubility of crystalline and amorphous polymers – Flory Huggins theory of polymer solution – nature of polymer molecules in solution – viscosity of polymer solution – osmotic pressure – swelling of polymers – fractionation of polymers – measurement of molecular mass; end group analysis, colligative property measurements – concentration dependence of colligative properties – vapour pressure lowering – osmotic pressure measurements – light scattering method – ultra centrifugation – solution viscosity and molecular size – empirical correlation between intrinsic viscosity and molecular size of polymer structures – gel

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UNIT – III POLYMERIZATION PROCESSES 18 Hours

Polymerization in homogenous and heterogeneous systems – bulk polymerization and polymer precipitation – suspension and emulsion Polymerization. Gas phase polymerization -solid phase polymerization. Types of polymer degradation; thermal and mechanical degradation – degradation by ultra sonic waves and by high energy radiation – photo degradation – oxidative and hydrolytic degradation – biodegradation of polymers

Polymer reactions; basic principles – molecular and chemical groups – reactivity of functional groups – post reactions of polymers – chain extension, branching and crosslinking reactions – polymer analogous reactions – vulcanization – cure reactions – reaction leading to graft and block polymers – polymer blends – functionalization of polystyrene.

UNIT – IV	POLYMER	COMPOSITES	AND	18 Hours
	APPLICATIONS	OF SOME POLYME		

Polymer Composites: Conventional fillers, Polymer nano composites: Types of nano Sized Fillers, Advantages of Nanosized fillers. Conducting polymers: Different types of conducting polymers (Extrinsic and Intrinsic) - Mechanism of conduction- Properties and uses of polyaniline, polyacetylene, polypyrrole, poly thiophene. Biopolymers: Applications of Biopolymers in biomedical applications: drug carrier, polymers for surgery and plasma substitution. Polymers with piezo electric, pyro electric and ferroelectric properties. Uses of some miscellaneous polymers: ABS, Kelvar, polyamide, polyimide, butyl rubbers

- 1. F W Billmyer Jr, Text book of polymer sciences, Wiley Intersciences
- 2. George Odian, Principles of polymerization, third Ed John Wiley and Sons
- 3. P J Flory, Principles of polymer chemistry, Cornel University press, London
- 4. J A Brydson, Rubber Chemistry, Applied Sciences London
- 5. F Rodrigues, Principles of polymer system, MeGraw Hill Boom Company
- 6. J M C cowie, Polymer chemistry and physics of modern materials, International Text Book Company 38
- 7. J A Bridesson, Plastic materials, Newness Butterworth
- 8. R J Young, Introduction to polymer sciences, John Wiley and Sons
- 9. K J Saunders, Organic polymer chemistry, Chapman Hall
- 10. V R Gowrikr and others, Polymer science, New age
- 11. Elias, Macromolecules, Plenum Press
- 12. I M Cambell, Introduction to synthetic polymers, Oxford Scientific Publications

- 13. H R Allocock, F W Lampe, Contemporary polymer chemistry, Pearson
- 14. R B Symour and E C Carraher, Polymer chemistry, Marcel Dekker, Inc, Newyork 1992
- 15. G S Misra, Introduction to polymer chemistry, New AGE 16. Naren, Polymer as aids in organic chemistry, Academic Press London

MSCHE04E06 MATERIAL CHEMISTRY

Credits: 4 Time: 72 Hours

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

- CO 1: To have a basic and general understanding about materials and material science related to engineering
- CO 2: To study about various types of materials important in the context of industrial applications
- CO 3: To understand the chemistry particularly electrical, magnetic and structural aspects of ceramics, composite and materials for special purposes
- CO 4: To study about the mechanism of processing, formation, stability and bonding in various types of materials

Course Content

UNIT I MATERIALS AND MATERIAL SCIENCE 18 Hours

Introduction. Classification of materials. Functional classification. Classification based on structure. Properties of engineering materials – mechanical, thermal, electrical magnetic, chemical and optical properties. Technological properties of metals and alloys. Bearing materials – types of bearing materials, self lubricating and porous bearing. Tool and dye materials – types of tool materials, die steels. Die – casting alloys – zinc base alloys, aluminum base alloys, copper base alloys. Magnetic materials – ferromagnetic, paramagnetic, diamagnetic and hard magnetic materials, ferrites. Refractory materials – introduction, molybdenum, tungsten and tantalum.

UNIT II MATERIALS FOR SPECIAL PURPOSES 18 Hours

Production of ultra pure materials – zone refining, vacuum distillation and electro refining. Ferroelectric and piezo electric material: general properties – classification of ferroelectric materials – theory of ferroelectricity – ferro electric domains – applications. Piezo electric materials and application Metallic glasses, preparation, properties and application.

Magnetic material – ferri and ferro magnetism – metallic magnets – soft, hard and super conducting magnets – ceramic magnets – low conducting and super conducting magnets Super conducting materials: Metallic and ceramic super conducting materials – theories of super conductivity – Meissner effect – high temperature super conductors, their structure and application.

Solar energy harvesting materials: Organic, Inorganic, hybrid photoconversion materials and devices

UNIT III CERAMIC MATERIALS 18 Hours

Ceramic materials – nature of ceramic materials, types of ceramics. Traditional and new ceramics – structure of ceramic – atomic interaction and types of bond – phase equilibria in ceramic systems – one component and multicomponent systems – use of phase diagrams in predicting material behavior- electrical, magnetic and optical properties of ceramic materials. Chemical reaction at high temperature and processing of ceramics – high temperature materials – crystalline ceramic materials – oxide, carbide, nitride, graphite and clay materials and their structures – polymorphism – nanocrystalline ceramic materials – structure and structural requirements for stability – mode of formation – silicate and nonsilicate glasses – Hydrogen bonded structures

UNIT IV COMPOSITE MATERIALS 18 Hours

Definition and classification of composites – fibers and matrices. Composite with metallic matrices – metal matrix composite processing, solid and liquid state processing, deposition. Ceramic matrix composite materials – introduction – processing of ceramic matrix composite – mixing and pressing, liquid state processing of ceramic matrix composites – liquid state processing, sol-gel processing, vapour deposition techniques, interfaces in composites, mechanical and micro structural characteristics Polymer composites, role of fiber and matrix in improving properties – bonding between fiber and matrix – critical fiber length in short fiber composites – failure mechanism in composite – composite fabrication techniques – open mould process, handy layup, vacuum bag moulding, centrifugal casting

- 1. W D Kingery, H K Dowen and R Duhlman, Introduction to ceramics, John Wiley
- 2. F H Nortion, Elements of ceramics, Addison-Wesley pub.co
- 3. C J Brinker and G W Sherer, Sol-gel science, the physics and chemistry of sol-gel processing, Academic press, Newyork 1990
- 4. A G Guy, Essentials of material Science, McGraw Hill
- 5. M J Starfield and Shrager, Introductory materials science, McGraw Hill
- 6. V Raghavan, A first course in material science, Prentice Hall Pvt Ltd, New Delhi
- 7. J H Shackelford, An introduction to material science for engineers, McMillian Pub.co, New Delhi
- 8. W F Smith, Foundation of material science and engineering, McGraw Hill Book Co 2000 23
- 9. M W Barsoum, Fundamentals of ceramics, McGraw Hill Book co 1997
- 10. S K Hagra Chaudhary, Material science and engineering, Indian book dist co. Kolkata

- 11. Sharp R S, Research Techniques in Nondestructive testing, Volume II, Academic PRESS, Newyork, 19973
- 12. J Kraut Kramer and H Kraut Kramer, Ultra sonic testing of materials, George Allen and Union limited, London, 1969
- 13. Analytical techniques for thin films in treatise on material science and technology, Vol
- 27, Acad, Press Inc, Newyork, 1991
- 14. S V Subramanian and E S Rajagopal, High temperature superconductor, Wile Eastern Ltd, 1988
- 15. M Tinkham, Introduction to superconductivity, McGraw Hill, Kogakusha, Ltd, 1975
- 16. A V Narlikar and S N Edbote, Superconductivity and superconducting materials, South Asian Pub, nEw Delhi 1983
- 17. Dekker, Electronic engineering materials, A J Prentice Hall of India Pvt Ltd, 1985
- 18. C M Srivastava and C Srinivasan, Science of engineering materials, Wiley Eastern Ltd 1987
- 19. Azaroff and Brophy, Electronic processing materials, McGraw Hill 1985
- 20. K K Chowla, Composite materials, Springer-Verlag, NY, 1987
- 21. F R Jones, Handbook of [polymer fiber composite, Longman Scientific and tech, 1994

MSCHE03&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
- 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.

MSCHE03&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----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, ¹H NMR, ¹³C NMR, and Mass spectra. (15 simple compounds only) like Phenol, Benzophenone, Acetophenone, Acetone, benzoic acid, Benzamide, aniline, α-naphthol, glucose, benzaldehyde, acetaldehyde etc.

[A minimum of 16 experiments to be recorded]

REFERENCES

- 1. A I Vogel, A Textbook of practical organic chemistry, Longman
- 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
- 8. Spectrometric Identification of Organic Compounds, Robert M. Silverstein, Francis X. Webster, David J. Kiemle, David L. Bryce, Wiley.
- 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.

MSCHE03&04C17: PHYSICAL 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. 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 K₂Cr₂O₇ (or KMnO₄)

Simultaneous determination of Mn and Cr in a solution of KMnO₄ and K₂Cr₂O₇

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 H₂O and NH₃ 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
- 2. A M James, Practical physical chemistry, J A Churchill
- 3. H H Williard, L L Merit, and J A Dean, Instrumental methods of analysis, Affiliated East West Press
- 4. D P Shoemaker and C W Garland, Experimental physical chemistry, McGraw Hill
- 5. J B Yadav, Advanced practical physical chemistry, Goel Publishers
- 6. B Viswanathan, P S Raghavan, Practical physical chemistry, Viva Books Pvt Ltd
- 7. V D Athawale Parul Mathur, Experimental physical chemistry, New Age International Publishers
- 8. A Findlay and J A Kitchener, Practical physical chemistry, Longmann
- 9. J. Foresman & Aelieen Frisch, Exploring Chemistry with Electronic Structure Methods,

Gaussian Inc., 2000.

- 10. David Young, Computational Chemistry- A Practical Guide for Applying Techniques to Real-World Problems", Wiley -Interscience, 2001.
- 11. http://classic.chem.msu.su/gran/gamess/index.html

MODEL QUESTION PAPER

I Semester M.Sc. Degree (C.B.C.S.S. - OBE –Regular)

Examination, October 2023

(2023 Admission) CHEMISTRY

MSCHE01C01: THEORETICAL CHEMISTRY I

Time: 3 hours Max marks: 60

SECTION A

Answer any 5 questions. Each question carries 3 mark.

 $(5\times3 = 15 \text{ marks})$

- 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.

 $(3\times6=18 \text{ marks})$

- 7. What are eigen functions and eigen values? Show that e^{ikx} is an eigen function of the momentum operator $P^{x} = i\hbar d/dx$. 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.

 $(3\times9=27 \text{ marks})$

- 12. Give the postulates of quantum mechanics
- 13. Set up the Schrodinger 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) Be₂ (ii) NO (iii) LiH
- 16. Setup the Hückel secular equation for cyclo butadiene , calculate the energies of the π orbitals and determine the delocalisation energy.

Model Question Paper

MSCHE01&02C05: INORGANIC CHEMISTRY PRACTICAL-I

..... on a separate sheet of paper. (3 Marks)

Record (Minimum 16 Experiments) (5 Marks)

5.

Model Question Paper

MSCHE01&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 MSCHE01&02C07: PHYSICAL CHEMISTRY PRACTICAL – I

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I ime	6	Hours
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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 the composition 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

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M Sc IV Semester Examination March 20--MSCHE03&04C15 Inorganic Chemistry Practical II

Time: 6 h	ours Max Marks: 40
·	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 containingg of ferric alum. Volumetry – 20 marks, Colorimetry -10 marks
	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

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MSc IV Semester Practical Examination March 20--

Time: 6 Hrs MSCHE03&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

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MSc IV Semester Practical Examination March 20--

Time: 6 Hrs MSCHE03&04C16 Organic Chemistry Practical II

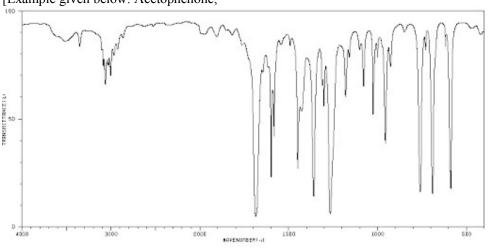
Max. Marks. 40

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