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)

2023

INDEX

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 Ia^{n} 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.

Semester	Paper Code	Title	Hrs /wk	Exam Duration	Marks for ESA	Marks for CA	Total	Credit
I	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
	MSCHE01C04	Physical Chemistry - I	4	3	60	15	75	4
	MSCHE01C05	Inorganic Chemistry Practical - I	3	Carried over to semester - II				
	MSCHE01C06	Organic Chemistry Practical - I	3	Carried over to semester - II				
	MSCHE01C07	Physical Chemistry Practical - I	3	Carried over to semester - II				
		Total :	25		240	60	300	16
II	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
	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
III	MSCHE03O01/02/03	Open Elective Paper I* (Multidisciplinary)	4	3	60	15	75	4
	MSCHE03C12	Inorganic Chemistry III	4	3	60	15	75	4
	MSCHE03C13	Organic Chemistry - III	4	3	60	15	75	4
	MSCHE03C14	Physical Chemistry - III	4	3	60	15	75	4
	MSCHE03C15	Inorganic Chemistry Practical - II	3	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 semester - IV				
	MSCHE03C18	Industrial Visit/Institutional Visit/Internship		Carried over to semester - IV				
		Total :	25		240	60	300	16
IV	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
	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)			40	10	50	4
		Total :	25		360	90	450	26

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

Semesterwise Split-up of Marks

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

6.3 Elective Papers: The M. Sc. 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
III	I (Open Elective/ Multidisciplinary	MSCHE03O01	Food Chemistry
		MSCHE03O02	Environmental Chemistry and Disaster Management
		MSCHE03O03	Medicinal Chemistry
IV	II	MSCHE04E01	Interdisciplinary topics and instrumentation techniques
		MSCHE04E02	Computational Chemistry
		MSCHE04E03	Biochemistry
IV	III	MSCHE04E04	Nanomaterial Chemistry
		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 IV^{th} semesters and the report should be submitted during IV^{th} semester practical examination along with project evaluation / Viva voce.

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

6.6 Continuous assessment

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

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

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

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

6.7 Grading system

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

GRADING PATTERN

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

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

6.8.1. Arrangement of contents shall be as follows:

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

6.8.2. Page dimension and typing instructions:

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

6.8.3. Bonafide certificate shall be in the following format

CERTIFICATE

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

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

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

DECLARATION

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

Date: Signature and name of the student

7. PATTERN OF QUESTION PAPERS

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

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

The distribution of questions will be as follows

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

SEMESTER-1		
MSCHE01C01: THEORETICAL CHEMISTRY - I		
Credit: 4		**TIME: 72 HOURS**

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

CO 1. Understand and examine the basic principles of Quantum Mechanics

CO 2. Apply the postulates of quantum mechanics to simple systems

CO 3. Make use of the approximation methods to calculate the properties of simple systems

CO 4. Demonstrate the principles of chemical bonding in diatomic and polyatomic molecules

CO 5. Apply HMO theory to simple conjugated systems

Course Content

UNIT -1	QUANTUM MECHANICS-I	18 Hours

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

UNIT – II	QUANTUM MECHANICS – II	18 Hours

Translational motion: Particle in a one-dimensional box-complete treatment – particle in a three-dimensional box (rectangular and cubical box) – degeneracy. Quantum mechanics of vibrational motion One-dimension Harmonic oscillator – complete treatment – Hermite polynomials – Recursion formula- comparison of classical and quantum mechanical results. Quantum Mechanics of rotational motion: Particle on a ring (Planar rigid rotator)- Particle on a sphere (Nonplanar rigid rotator) – the wave function in spherical polar co-ordinates – complete treatment – Legendre polynomial –Rodrigue's formula- spherical harmonies – wave function in the real form- polar diagrams- Quantum mechanics of Hydrogen like atoms: potential energy of hydrogen-like atoms – the wave equation in spherical polar co-ordinates – solution of the R, θ, ϕ equations – Laguerre polynomials – associated Laguerre polynomials – Discussion of the wave functions –radial function, radical distribution function and angular function and their plots– orbitals and orbital diagrams – their significance.		
UNIT – III	**QUANTUM MECHANICS – III**	18Hours
Need of approximate methods in quantum chemistry: variation method – variation theorem with proof –illustration of variation theorem using a trial function [e.g., x (a-x)] for the particle in a 1D-box and using the trial function e -αr2 for the hydrogen atom, variation treatment for the ground state of helium atom; Perturbation method: time-independent first-order correction to the energy and wave function, second-order correction to energy– illustration by application to particle in an ID-box with slanted bottom, perturbation treatment of the ground state of the helium atom. Electron spin and atomic structure: spin functions and operators –spin-orbit interactions – Angular momentum – commutation relations – operators Term symbols – Russel – Saunder's terms and coupling schemes – introduction to SCF methods – Hartree and Hartree – Fock's SCF.		
UNIT – IV	**CHEMICAL BONDING**	**18 Hours**
Born – Oppenheimer approximation – essential principles of the MO method – MO treatment of Hydrogen molecule and the H_2+ ion – valence bond treatment of the ground state of hydrogen molecule – MO treatment of homonuclear diatomic molecules (quantitative) – Li_2, Be_2, N_2, O_2, O_2+, O_2-, F_2 and heteronuclear diatomic - LiH, CO, NO, HF – theory of chemical bonding for polyatomic molecules – *Ab initio* calculations – basic principles — basis sets – STO and GTO –Spectroscopic term symbols for diatomic molecules.		

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

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– 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 SOLVENTS	18 Hours

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

Superacids and bases – Types, examples, and applications

Classification of solvents – properties of 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 COMPOUNDS**	**18 Hours**
The neutral boron hydrides – structure and bonding topological approach to boron hydride structure – Styx number – synthesis and reactivity of neutral boron hydrides. Importance of icosahedral framework of boron atoms in boron chemistry – closo, nido, and arachno structure – Wades rule – mno rules Carboranes– Structure and classification - preparation and properties of dicarba-closododecaboranes ($C_2B_{10}H_{12}$ - ortho, meta, and para) - metallocarboranes – preparation and structure of metallo carboranes of Fe & Co Phosphorous sulphides – P_4S_3, P_4S_5, P_4S_7, and P_4S_{10} – preparation, properties, structure, and uses. The phosphazenes (phosphonitrilic halides) Sulphur nitrogen compounds – S_2N_2 and S_4N_4 – Polythiazyl, other S_XN_Y compounds. Their preparation properties, and structure. Poly acids - Iso poly and heteropoly acids of Mo & W elements – Structure and formation		

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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 REARRANGEMENTS**	**18 Hours**

Structure, formation, and properties of carbenes, nitrenes, and arynes – singlet and triplet carbenes,

nitrenes and arynes, Carbon free radicals: structure, formation, and stability. Structure, stability, and formation of Ylides, Enamines, 1,3-dithiane, Benzynes, and Enolates. Molecular rearrangement mechanism. Carbon to carbon migration: Wagner Meerwein, Pinacol, Wolff, Benzilic acid, Demjanove, Dienone-phenol, Hoffmann-Martius. Carbon to nitrogen migration: Hofmann, Curtius, Schmidt, Lossen, Beckmann. Migration to electron-rich carbon: Wittig, Wittig-Hormer, Favorski, Stevens, Neber Orton, Bamberger. Migration to electron-deficient oxygen: Baeyer, villager, Darkin reaction. Aromatic rearrangements: benzidine, Fries, Von-Richter Sommlet-Hauser.		
UNIT- II	**SUBSTITUTION AND ELIMINATION REACTIONS**	**18 Hours**
Aliphatic nucleophilic substitution reactions – saturated and unsaturated systems – Mechanism of nucleophilic substitution – SN2, SN1, SNi, SET. Neighbouring group participation – non-classical carbocations. Substitution at allylic and vinylic carbon atoms. Effect of substrate structure, attacking nucleophile, leaving group, and reaction medium on reactivity and regioselectivity. Aliphatic Electrophilic substitutions: SE1 SE2 and SEi mechanisms with suitable examples. Elimination Reaction: Mechanistic and stereochemical aspects of E1, E2, and E1cB eliminations. The effect of substrate structure, base, leaving group, and reaction medium on elimination reactions. Elimination reaction in 4-t-Butylcyclohexyl tosylate (cis and trans), 2-Phenylcyclohexanol (cis and trans), Menthyl and neomenthyl chlorides, and benzene hexachlorides. Saytzev vs. Hofmann elimination, Bredt's rule, α- elimination, pyrolytic syn elimination (Ei) – Chugaev reaction, and Cope elimination. Dehydration of alcohols, Dehalogenation of vicinal dihalides, and Peterson elimination.		
UNIT- III	**AROMATICITY AND AROMATIC REACTIONS**	**18 Hours**
MO description of aromaticity and antiaromaticity. Homoaromaticity. Aromaticity of annulenes and heteroannulenes, fused ring systems, fulvenes, fulvalenes, azulenes, pentalenes, and heptalenes. mesoionic compounds, metallocenes, cyclic carbocations, and carbanions. Effect of delocalized electrons on pKa. Aromatic Electrophilic Substitution: Arenium ion mechanism, substituent effect on reactivity in mono and disubstituted benzene rings, *ortho/para* ratio, *Ipso* substitution. Relationship between reactivity and selectivity. Aromatic Nucleophilic substitution: Addition-elimination (SNAr) mechanism, elimination-addition (benzyne) mechanism, *cine* substitution, SN1 and SRN1 mechanism. The effect of		

substrate structure, nucleophile, and leaving group on aromatic nucleophilic substitution. Nucleophilic Substitution of Pyridine-Chichibabin Reaction.		
UNIT- IV	**PHOTOCHEMISTRY**	**18 Hours**
Photochemical excitation of molecules, spin multiplicity, Jablonski diagram, photosensitization, and quenching. Photochemistry of carbonyl compounds: Norrish type- I cleavage of acyclic, cyclic, and β, γ- unsaturated carbonyl compounds. Norrish type- II cleavage, photo reduction, photoenolization. Photocyclo- addition of ketones with unsaturated compounds: Paterno- Büchi reaction, photodimerization of α, β- unsaturated ketones, Photo rearrangements: Photo –Fries, di- π- methane, oxa di- π- methane, aza di- π- methane, lumi ketone rearrangements. Barton and Hoffmann- Loeffler- Freytag reactions. Photo isomerization and dimerization of alkenes, photo isomerization of benzene and substituted benzenes, and photo-oxidation. Photochemistry of vision and photosynthesis.		
REFERENCES: 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 9. I L Finar, Organic Chemistry Volume 2, Pearson Education. 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 EQUILIBRIA**	**18 Hours**

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

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

Phase equilibria: Phase rule -Physical equilibria involving phase transition-criteria for equilibrium between phase-Three component system- graphical representations-solid liquid equilibria Ternary solution with common ion-Hydrate formation-compound formation-liquid-liquid equilibria-one pair of partially miscible liquids-two pairs of partially miscible liquids-three pairs of partially miscible liquids.

UNIT-II	**ELECTROCHEMISTRY**	**18 Hours**

The nature of electrolytes– Ionic mobilities- ion activity- ion-ion and ion -solvent interaction. Equilibrium properties of electrolyte solutions. Electrolytes of the first and second kind, - Influence of pressure and temperature on ion conductance-Walden's equation- Abnormal ion conductance-Derivation of Debye-Huckel Onsager equation- the validity of Debye-Huckel-Onsager equation for aqueous and non-aqueous solution-Deviation from Onsager equation-Conductance ratio and Onsager equation-Dispersion of conductance at high frequencies-Triple ion conductance minima-Equilibria in electrolytes-Association constant Ion-association-dissociation constant--- Activities and activity coefficient in electrolytic solutions.-Debye-Huckel limiting law and its various form, qualitative and quantitative tests of Debye-Huckel limiting equation. Osmotic coefficient- solubility product principle-solubility in the presence of common ion-activity coefficient and solubility measurement.		
UNIT-III	**ELECTRODICS**	**18 Hours**
Liquid junction potential. The electrode double layer-electrode-electrolyte interface-Theory of multilayer capacity. Electric capillary Lippmann -potential, Membrane-potential. Butler Volmer equation for simple electron transfer reaction-Transfer coefficient- Exchange current density Rate constants- Tafel equation and its significance. Electrolytic polarization- dissolution and deposition potentials, concentration polarization. Decomposition voltage and its determination. Overvoltage - hydrogen and oxygen overvoltage, metal deposition over-voltage, and their determination. Theories of overvoltage. Cyclic Voltammetry- Theory and experimental setup, Cyclic voltammogram. Polarography- Principle and instrumentation Dropping mercury electrode- half-wave potential and Ilkovic equation.		
UNIT-IV	**APPLIED ELECTROCHEMISTRY AND CORROSION**	**18 Hours**
Energy storage devices: Batteries- Working of Lithium-ion battery. Basics of supercapacitors, Classification with examples. Electrostatic double layer capacitors (EDLC) and Psuedo capacitors-working and principle. **Corrosion**: Thermodynamics of corrosion and electrode potentials. EMF of a cell-measurement- emf calculation of half cell potential-Nernst equation. Basis of Pourbaix diagrams- Diagrams of water, Fe, and Al. Limitations of Pourbaix diagrams. Kinetics of corrosion- Polarization and corrosion rate. Measurement of corrosion rate. Measurement of polarization- causes of polarization. Calculation of IR drops in an electrolyte. Influence of polarization on corrosion rate. Polarization diagram of corroding metals. Calculation of corrosion rate from polarization data. Theory of cathode protection.		

Passivity.

REFERENCES

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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
11. G.M. Barrow- Physical Chemistry- Tata McGraw-Hill.
12. Duta K. Robin "Physical Chemistry" AbeBooks
13. Winston Revie and Herbert Uhlig, Corrosion and corrosion control:(Wiley) Edited by L. L. Shreir, G. T. Burstein, R. A. Jarman Corrosion ControlVolume2:
14. Fontana and Greene Corrosion Engineering:
15. What are batteries, fuel cells, and supercapacitors? *Chem Rev.2004,104,4245-4269*
16. Electrochemical methods: Fundamentals and application by Allen J. Bard and Larry R Faulkner.
17. Lithium-ion batteries basics and applications by Reiner Korthaneur.
18. Electrochemical supercapacitors: Scientific fundamentals and Technological applications, B.E. Conway.

SEMESTER – II

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, MATRICES**	**18 Hours**

Symmetry elements and symmetry operations in molecules –point groups and their symbols – Classification of point groups– Systematic identification of point groups- order of a group- finite, Infinite, abelian, non-abelian, cyclic, and non-cyclic groups – sub-groups- Mathematical groups and its properties- group multiplication tables of C_{2v}, $C_{2h,}$ and C_{3v} –Rearrangement theorem- classes in a group and similarity transformation – Matrices – addition and multiplication of matrices – the inverse of a matrix- the character of a matrix- block diagonalization – matrix notation of symmetry operations –General expression for the character of an operation- representation of groups – construction of representation using vectors and atomic orbital as the basis – Γcart, Representation generated by Cartesian coordinates positioned on the atoms of a molecule (H_2O and SO_2 as examples) -Γregular – reducible and irreducible representations – construction of irreducible representation by reduction.

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

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

Applications of Group theory- Applications to chemical bonding – construction of hybrid orbitals – BF_3 CH_4, PCI_5 as examples- Application to MO theory-. Group orbitals and their construction-Projection Operator method and pictorial method- Transition Moment Integral. Examples H_2O, $NH_{3,}$ and octahedral complexes (sigma bonding using the pictorial method)

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

UNIT – III	SPECTROSCOPY	18 Hours

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

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

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

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

UNIT –IV	SPECTROSCOPY II	18 Hours

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

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

REFERENCES

1. F A Cotton, *"Chemical Applications of Group Theory"* Wiley Eastern.
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
7. Barrow "*Molecular Spectroscopy,"* McGraw Hill.
8. P W Atkins *"Physical Chemistry*," ELBS
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 d^n ion. selection rules for d-d transitions – effect of spin-orbit coupling and vibronic coupling on electronic transitions - Orgel diagram of transition metal complexes(d^1 to d^9 configurations) Tanabe Sugano diagrams - Charge Transfer Spectra Magnetic behaviors – susceptibility, measurements – Gouy method diamagnetic corrections. Spin-only value – orbital contributions – spin-orbit coupling, ferro, and antiferro magnetic coupling – spin cross-over system – Temperature dependence of magnetic behaviour - Applications of magnetic measurements to structural determinations of transition metal complexes.		
UNIT – III	**COORDINATION CHEMISTRY III**	**18 Hours**
The reaction of metal complexes: Stability constants – chelate effect – Irwing-Willian order of stability. Factors affecting the stability of metal complexes. Determination of binary formation constants by pH meter and spectrophotometry – Job's Method - energy profile of a reaction Reaction of complexes: Ligand substitution reactions (Square planar and octahedral complexes). Rates of ligand substitutions, classification of mechanisms. The nucleophilicity of the entering group, The shape of the transition states, The activation of octahedral complexes, Base hydrolysis, stereochemistry, and Isomerisation reactions. A brief study of redox reaction – Outer sphere and Inner sphere mechanism – Marcus -Husch Theory		
UNIT– IV	**PHYSICAL TECHNIQUES IN INORGANIC CHEMISTRY**	**18 Hours**
Study of inorganic compounds by the following methods - Diffraction methods – X-ray diffraction, neutron diffraction UV, IR, Raman Spectroscopic Methods, Resonance technique – nuclear magnetic resonance, electron paramagnetic resonance, Mossbauer spectroscopy Ionization-based techniques – photon electron spectroscopy, x-ray absorption spectroscopy, mass spectrometry Chemical analysis – atomic absorption spectroscopy, CHN Analysis, X-ray fluorescence elemental analysis Magnetometry – electrochemical techniques		

REFERENCES

1. S F A Kettle, Coordination Chemistry, Thomas Nelson and Sons
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 ASYMMETRIC SYNTHESIS**	**18 Hours**
Molecules with C, N, S based chiral centers. Axial, planar, and helical chirality with examples of R and S nomenclature using Cahn-Ingold-Prelog rules. Optical purity, enantiomeric excess, and diastereomeric excess and their determination. Topicity and pro stereoisomerism, prochiral centre, enantiotopic, homotopic, diastereotopic hydrogen atoms. Asymmetric synthesis, need for asymmetric synthesis, stereoselectivity, and stereospecificity. Strategies in Asymmetric Synthesis: Chiral pool: Amino acids in the synthesis of benzodiazepines-conversion of L-tyrosine into L-Dopa; synthesis of beetle pheromone component (S)- (–)-ipsenol from (S)-(–)-leucine, Carbohydrates – (R) Sulcatol from 2-deoxy-D-ribose. Cram's rule, Cram's chelation control, Prelog's rule, and Felkin-Anh model.		
UNIT III	**PERICYCLIC REACTIONS**	**18 Hours**
Symmetry properties of MOs – LCAO-MO theory of simple conjugated polyenes and cyclic polyenes – classification of pericyclic reactions- electrocyclic, cycloaddition, sigmatropic, chelotropic, and group transfer reactions. Mechanism and stereo course of electrocyclic, cyclo addition, and sigmatropic reactions. Analysis of electrocyclic, cyclo addition, and Sigmatropic reactions by FMO, Woodward-Hoffmann Selection Rule, and Huckel-Mobius Method. Correlation diagram approach for electrocyclic, and cyclo addition reactions. Study of Electrocyclic Reactions: Nazarov cyclization. Study of Cycloaddition reactions: Stereo and Regiochemistry of Diels –Alder reaction, Intramolecular, Asymmetric, and retro Diels –Alder reaction. 1,3-dipolar cycloaddition, Ketene [2+2] cycloaddition. Sigmatropic reaction: [3,3] Cope rearrangement, Oxy-cope rearrangement, Aza cope rearrangement, classes, thia-claisen rearrangement, Fluxional molecules. [2,3] sigmatropic rearrangement, [5,5] sigmatropic rearrangement. Group transfer reactions: inter and intramolecular ene reactions, Carbonylene reaction, metallo-ene reaction. Chelotropic reactions:		

(2+2) chemotropic cycloaddition, (4+2) chelotropic cycloaddition, stereochemistry of chelotropic reactions		
UNIT -IV	**ORGANIC REACTIONS AND REAGENTS**	**18 Hours**
Mannich, Simon-Smith, Heck, reactions. Michael, Prevost, and Woodward hydroxylation of alkenes, Shapiro reaction, Sharpless asymmetric epoxidation, ring formation by Dieckmann, Thorpe, and Acyloin condensation. Robinson ring annulations, reduction, and oxidation in synthesis – catalytic hydrogenation. Alkali metal reduction. Birch reduction. Wolff-Kishner reduction, Huang-Milon modification. Clemmenson reduction. LAH, DIBAL, sodium borohydride as reductance. Oppenauer oxidation. HIO_4, OsO_4, and mCPBA and their applications. Synthetic applications of the following reagents – Gillman's reagent, LDA, 1, 3 dithianes, DDQ, DDC, SeO_2, Bakers yeast, NBS, Wilkinsons's catalyst. Asymmetric reductions using BINAL-H. Asymmetric hydroboration using IPC2BH and IPCBH2. Reduction with CBH reagent.		

REFERENCES

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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.
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12. J. Clayden, N. Greeves, S. Warren, P. Wothers, Organic Chemistry, Oxford University Press, 2004.
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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 AND QUANTUM STATISTICS**	**18 Hours**
Partition function and thermodynamic functions- Partition function and equilibrium constants - Equation of state – Sackur Tetrode equation- Statistical formulation of the third law of thermodynamics. Need for quantum statistics, Bose-Einstein statistics: Bosons-Bose Einstein distribution law, Bose-Einstein condensation, liquid helium, Fermi- Dirac statistics: Fermions- Fermi- Dirac distribution law, application to electrons in metals- Thermionic emission. Comparison of three statistics.		
UNIT-III	**IMPERFECTIONS IN SOLIDS AND**	**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 TiO_2(anatase and rutile structure only)

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

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

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

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

Magnetic properties- diamagnetism- 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.

REFERENCES

1. M.C. Gupta-"Elements of Statistical Thermodynamics-New Age International.
2. L.K Nash-"Elements of Statistical Thermodynamics-Addision Wesley publishing.
3. Kistinand Sorfuran-"A course on statistical thermodynamics"-Academic 1971.
4. D.A.McQuarie-"Statistical thermodynamic"-HarperandRow1973.
5. D.K. Chakraharth-"Solid state chemistry"-New age publication.
6. I.V.Azaroof-"Introduction to solids"-McCrawHil.
7. Lesley E. Smart and Elaine A. Moore. "Solid state chemistry an introduction" Third edition, 2005. Taylor and Francis group.
8. A.R.West, Solid State Chemistry and its Applications, (1984) John Wiley and Sons, Singapore
9. UriShmueli. "Theories and techniques of crystal structure determination" Oxford University Press,

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11. Molewyn Hughes-"Physical chemistry"-Pergamon press. 24. S. Glasstone and H.S. Taylor-"Treatise of Physical Chemistry"-Dvan Nostrand.
12, Feridoun Samavat*, Mohammad Hossein Tavakoli, Safdar Habibi, Babak Jaleh, Parisa Taravati Ahmad, Open Journal of Physical Chemistry, 2012, 2, 7-14

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

Credit: 2		**TIME:108 Hours**

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

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

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

CO 3: Analyze metal ions using the volumetric method

CO 4: Analyze water quality parameters like hardness and DO

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

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

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

Course Content:

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

(Ist and 2nd SEMESTER)		
Credit: 2		**Time: 108 Hours**

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

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

CO 2. Estimate concentration and molecular weights using cryoscopic methods

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

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

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

Course Content

1) Conductivity experiments

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

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

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

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

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

2. Solubility and Heat of solution

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

3. Molecular weight determination

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

4. Cryoscopic study

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

5. Refractometry

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

6. Viscosity

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

7. Potentiometry

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

8. Phase rule

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

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

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

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

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

REFERENCES

1. A Findlay and J A Kitchener, Practical physical chemistry, Longman
2. F Daniels and J H Mathews, Experimental physical chemistry, Longman
3. A M James, Practical physical chemistry, J A Churchill
4. H 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 AND RELATED COMPOUNDS	18 Hours

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

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

Thermodynamic aspects of extraction. Ellingham diagrams – Lattimer and Frost diagrams. Extraction, properties and uses of thorium, uranium, and plutonium. Beach sands of Kerala – important components and their separation from-monazite & 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 O_2 transport-hemerythrin and haemocyanins,. Electron transfer proteins-cytochromes, iron-sulphur proteins (Bacterial Ferredoxins, Rubredoxin). Metalloproteins as enzymes– carboxy peptidase, carbonic anhydrase, alcohol dehydrogenase, superoxide dismutase -Structure and Mode of Action, Biomineralization Process. Therapeutic uses of Metals- Metal complexes in cancer therapy, rheumatoid arthritis, imaging agents and chelation therapy		

REFERENCES

1. Alan G Sharp – Inorganic chemistry third edition, Pearson
2. J E Huheey, E A Keiter and R L Keiter, Inorganic chemistry principles of structure and reactivity, Pearson education
3. D F Shriver and P W Atkins, Inorganic Chemistry, Oxford University Press
4. Sathya prakash, G D Tuli, S K Basu and R D Madan, Advanced inorganic chemistry Volume II, S Chand Publication
5. Cotton, Wilkinson, Bachmann, Advanced inorganic chemistry, Wiley India Pvt Ltd

6. B Douglas D MeDaniel and J Alexander, Concepts and models of inorganic chemistry 3rd edition, John Wiley and Sons Inc
7. S J Lippard and J M Berg, Principles of bioinorganic chemistry, University Books California
8. David E Fenton, Bio coordination chemistry, Oxford University Press
9. I Bertni, H B Grey, S J Lippard and J S Valentine, Bio inorganic chemistry, Viva Books Pvt Ltd, New Delhi
10. DMP Mingo's Essential Trends in inorganic chemistry, Oxford University Press
11. K Hussain Reddy Bioinorganic chemistry New age international
12. Indrajith Kumar, Organometallic compounds, Pragati Prakashan Meerut
13. R C Melhotra and A Singh, Organometallic Chemistry, New age international
14. M.N. Hughes: Inorganic Chemistry of Biological Processes, (2ndedn.) Wiley, 1988.
15. K. Hussain Reddy, Bioinorganic Chemistry - New Age International Ltd. (2003).
16. R.W. Hay, Bioinorganic Chemistry - Ellis Horwood Ltd., (1984) 6. Asim K Das, Bioinorganic chemistry, Books & Allied (P) Ltd.
17. Gupta, B.D, Elias, A J; Basic Organometallic Chemistry, Concepts, syntheses and applications, 2nd edn, Universities Press, 2013.
18. Organometallics, Elschenbroich,Ch, 3 rd edn, Wiley VCH, 1989.
19. Organometallics and catalysis An introduction. Bochmann, M, 1st edn, Oxford, 2014
20. The organometallic chemistry of the transition metals, Crabtree R H, 6th edn, Wiley, 2014.
21. Organotransition metal chemistry: From bonding to catalysis, Hartwig, J.F, 1st edn, University science books, 2010.

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 absorption – the chromophore concepts – theory of electronic spectroscopy laws of

light absorption – Beer-Lambertz law – solvents and solutions – effect of solvent polarity on UV absorption – electronic transition in enes, enones and arenes, Woodward Fieser rule Empirical rules for calculating λmax of dienes, enones and benzene derivatives. instrumentation and sampling. IR spectroscopy – factors influencing vibrational frequencies – Conjugation, coupling, electronic, steric, ring strain and hydrogen bonding. principles of characteristics frequency in IR- application of IR – identity by finger printing – identification of functional groups and other structural features by IR – Hydrogen bonding and IR bands – Instrumentation and sampling techniques – FTIR and its instrumentation.		
UNIT II	**NMR SPECTROSCOPY IN ORGANIC CHEMISTRY**	**18 Hours**
1HNMR: Chemical shift, factors influencing chemical shift, electronegativity, shielding and deshielding, van der Walls deshielding, anisotropic effect, magnetic anisotropy, H-bonding, diamagnetic and paramagnetic anisotropies. Chemical shift values of protons in common organic compounds, chemical, magnetic and stereochemical equivalence. Spin – spin coupling, types of coupling, coupling constant, factors influencing coupling constant, – analysis of 1st order spectra, spectral interpretation using actual spectra taken from standard texts . Simplification of NMR spectra use of high field NMR – shift reagents, chemical exchange and double resonance – NOE spectra, heteronuclear coupling. Introduction to COSY, HMBC, HMQC spectra. 13C NMR: General considerations, comparison with PMR, factors influencing carbon chemical shifts, carbon chemical shifts and structure-saturated aliphatics, unsaturated aliphatics, carbonyls, and aromatics. Off-resonance and noise decoupled spectra, Introduction to DEPT, INEPT, INADEQUATE.		
UNIT III	**ORGANIC MASS SPECTROSCOPY**	**18 Hours**
Instrumentation – EI, CA, FAB, Electro spray and MALDI ion sources – magnetic high resolution (double focusing), TOF and Quadropole mass analysers – isotope abundance - molecular ion – molecular mass from molecular ion – meta stable ion – significance of meta stable ion – fragmentation process – basic fragmentation types and rule – factors influencing fragmentation – fragmentation associated with functional groups – alkanes, alkyne, halides, alcohols, ethers, carbonyl compounds, carboxylic acids, amides – characteristic fragmentation modes and Mc Lafferty rearrangement –GCMS, LCMS.		
UNIT IV	**HETEROCYCLICS AND BIOMOLECULES**	**18 Hours**
Nomenclature of heterocycles, replacement and systematic nomenclature, Hantzsch-Widman system for monocyclic compounds. Synthesis and reactions of the following four membered heterocycles – oxitanes, azetidines and thietanes; five membered heterocylces – imidazoles, pyrazolines, six		

membered heterocycles –pyrimidines and pyrazines; seven membered heterocycles – azepines, oxepines and thiepines – fused heterocycles; indole, quinoline, isoquinoline and coumarins.

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

REFERENCES

1. W Kemp, Organic spectroscopy, Palgrave
2. J March, Advanced organic chemistry, Wiley
3. R O C Norman and A Coxon, 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

MSCHE03C14 : 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

<table>
<tr><td colspan="3">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.</td></tr>
<tr><td>UNIT – II</td><td>KINETICS AND CATALYSIS</td><td>18 Hours</td></tr>
<tr><td colspan="3">Chain reaction–stationary and non-stationary chain- explosion and explosion limits-free radical and chain reaction- steady state treatment- kinetics of H_2-CI_2 and H_2-Br_2-decomposition of acetaldehyde-Rice Herzfeld mechanism- Branching chain-H_2O_2 reaction-Semenov Hinshelwood mechanism of explosive reaction. Acid – base catalysis-specific and general catalysis-prototropic and protolytic mechanism- examples-Acidity function. Enzyme catalysis-Michaelis-Menten equation derivation-effect of pH and temperature. Reaction in solution- Factors determining reaction rates in solution–Effect of pressure-dielectric constant-ionic strength-cage effect-Bronsted- Bjerrum equation-Primary and secondary kinetic salt effect-Influence of solvent on reaction rate-Hammet & Taft equation.</td></tr>
<tr><td>UNIT – III</td><td>SURFACE CHEMISTRY</td><td>18 Hours</td></tr>
<tr><td colspan="3">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.</td></tr>
<tr><td>UNIT – IV</td><td>COLLOIDS</td><td>18 Hours</td></tr>
<tr><td colspan="3">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</td></tr>
</table>

dynamics- diffusion coefficient and molecular size determination from diffusion co-efficient.

REFERENCES

1. K.J. Laidler-“Chemical kinetics” Pearson Education
2. S.Glasstone,K.J.LaidlerandEyring-“TheTheoryofrateprocesses”-McGrawHils
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 AND FLAVOR ENHANCERS**	**18 Hours**

Introduction, Historical development of food chemistry. Food Constituents-Carbohydrates-classification and physical properties, changes of carbohydrates on cooking. Lipids-occurrence in food and composition, fats and oils, Hydrogenation, Rancidity, reversion, rendering, extraction and refining. enzymes- classification and properties, vitamins-fat and water soluble, peptides, amino acids and protein-physical properties. Protein sources, Protein denaturation. Determination of

<table>
<tr><td colspan="3">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.</td></tr>
<tr><td>UNIT–II</td><td>CHEMISTRY OF FOOD: ADDITIVES, PRESERVATIVES, AND CONTAMINATION</td><td>18 Hours</td></tr>
<tr><td colspan="3">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.</td></tr>
<tr><td>UNIT–III</td><td>CHEMICAL COMPOSITION OF FOOD AND NUTRITIONAL ASPECTS</td><td>18 Hours</td></tr>
<tr><td colspan="3">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</td></tr>
<tr><td>UNIT – IV</td><td>ANALYTICAL METHODS AND NANOTECHNOLOGY IN FOOD</td><td>18 Hours</td></tr>
<tr><td colspan="3">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.</td></tr>
<tr><td colspan="3">REFERENCES
1. Mousumi Sen, Food Chemistry: The Role of Additives, Preservatives and Adulteration
2. Peter C. K. Cheung, Bhavbhuti M. Mehta, Handbook of Food Chemistry.</td></tr>
</table>

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
MSCHE03O02: 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 POLLUTION**	**18 Hours**

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 SO_2, NO_X, CO, H_2S, smoke, hydrocarbons on human and plant systems. Cause and consequence of acid rain, green house effect, ozone depletion and photochemical smog. Air pollution control method. Air pollution accident – Bhopal tragedy

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

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

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

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

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

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

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

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MSCHE03O03: 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, MECHANISM, AND SYNTHESIS**	**18 Hours**

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**	**18 Hours**
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-INFLAMMATORY AGENTS**	**18 Hours**
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.		

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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 Fe^{2+} and Fe^{3+}		

REFERENCES

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2. P T Anastas and J C Warner Green Chemistry Oxford
3. G A Ozin, A C Arsenault, Nano chemistry RSC
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5. V S Muralidharan, A Subramania, Nano science and technology, Ane books
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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.		
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4. David Young, *Computational Chemistry- A Practical Guide for Applying Techniques to Real World Problems*, Wiley -Interscience
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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 METABOLISM**	**18 Hours**

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.

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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 NANOMATERIALS	18 Hours

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

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.		

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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 CHEMISTRY**	**18 Hours**
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		

permeation chromatography in the fractionation of polymers		
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 APPLICATIONS OF SOME POLYMERS**	**18 Hours**
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		

REFERENCES

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 modem 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 an d 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		

REFERENCES

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2. F H Nortion, Elements of ceramics, Addison-Wesley pub.co
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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
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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
2) D M Adams and J B Raynor, Advanced practical inorganic chemistry, CRC Press, New York
3) W L Jolly, Preparative Inorganic reactions, Interscience Publishers, New York
4) Textbook of Nanoscience and Nanotechnology, 2012 McGraw Hill Education (India) Private Limited By T Pradeep
5) Springer Handbook of Nanomaterials, by Robert Vajtai
6) *Solution-Grown Zinc Oxide Nanowires, by Lori E. Greene, Benjamin D. Yuhas, Matt Law, David Zitoun, and Peidong Yang*, Inorg. Chem. 2006, 45, 7535−7543.*

MSCHE03&04C16: ORGANIC CHEMISTRY PRACTICAL – II
(3^{rd} and 4^{th} SEMESTER)

Credit: 2		Time: 108 Hours

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

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

CO 2. Synthesize and purify organic compounds

CO 3. Develop skills in chromatographic techniques.

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

Course Contents:

1) Quantitative analysis and Extraction of natural products:

Estimation of the following

i) Phenol (Using bromate-bromide mixture)

ii) Aniline (Using bromate-bromide mixture)

iii) Reducing sugars (using Fehling solution)

iv) Iodine value of vegetable oil

v) Saponification of vegetable oil

vi) Estimation of ascorbic acid (Colorimetric method)

Extraction of natural compounds

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

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

a) Preparation of p-nitroaniline from acetanilide:

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

b) Preparation of Methyl orange from aniline:

Aniline---sulphanilic acid---methyl orange

c) Preparation of p-aminoazobenzene from aniline:

Aniline---diazoaminobenzene---p-aminoazobenzene

d) Preparation of m-nitroaniline from nitrobenzene:

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

e) Preparation of Benzilic acid benzoin:

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

f) Preparation of Benzanilide from benzophenone:

benzophenone---benzophenone oxime—benzanilide

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

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

h) Preparation of caprolactam from cyclohexanone:

Cycohexanone----cyclohexanone oxime---Caprolactum

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

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

3) Chromatographic Techniques:

Practical application of TLC:

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

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

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

4) Spectral evaluation of organic compounds:

Solving spectral problems from the standard textbooks by providing IR, ^{1}H NMR, ^{13}C NMR, and Mass spectra. (15 simple compounds only) like Phenol, Benzophenone, Acetophenone, Acetone, benzoic acid, Benzamide, aniline, α-naphthol, glucose, benzaldehyde, 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, 4^{th} 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 $K_2Cr_2O_7$ (or $KMnO_4$)

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

Investigation of complex formation between Fe(III) and thiocyanate

5) Spectral analysis calculations

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

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

6) Computational Chemistry Calculations

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

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

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

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

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

[A minimum of 16 experiments to be recorded]

REFERENCES

1. F Daniels and J H Mathews, Experimental physical chemistry, Longmann
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
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MODEL QUESTION PAPER
I Semester M.Sc. Degree (C.B.C.S.S. - OBE –Regular)
Examination, October 2023
(2023 Admission)
CHEMISTRY
MSCHE01C01: THEORETICAL CHEMISTRY I

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

SECTION A

Answer any 5 questions. Each question carries 3 mark.

(5×3 = 15 marks)

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

SECTION B

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

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

SECTION C

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

12. Give the postulates of quantum mechanics
13. Set up the 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) Be_2 (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

Time: 6 Hours

Max Marks:40

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

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

Model Question Paper

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

Time: 6 Hours

Max Marks:40

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

2. Determine the solid-liquid equilibrium for the binary system formed by the two substances A and B by the cooling curve method. Use the phase diagram to determine 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

KANNUR UNIVERSITY

M Sc IV Semester Examination March 20--

MSCHE03&04C15 Inorganic Chemistry Practical II

Time: 6 hours Max Marks: 40

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

   Volumetry – 20 marks, Colorimetry -10 marks

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

   5 marks

For procedure writing any one of the following may be given

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

Record……………………………………………………………….. 5 marks.

KANNUR UNIVERSITY
MSc IV Semester Practical Examination March 20--
Time: 6 Hrs 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

KANNUR UNIVERSITY

MSc IV Semester Practical Examination March 20--

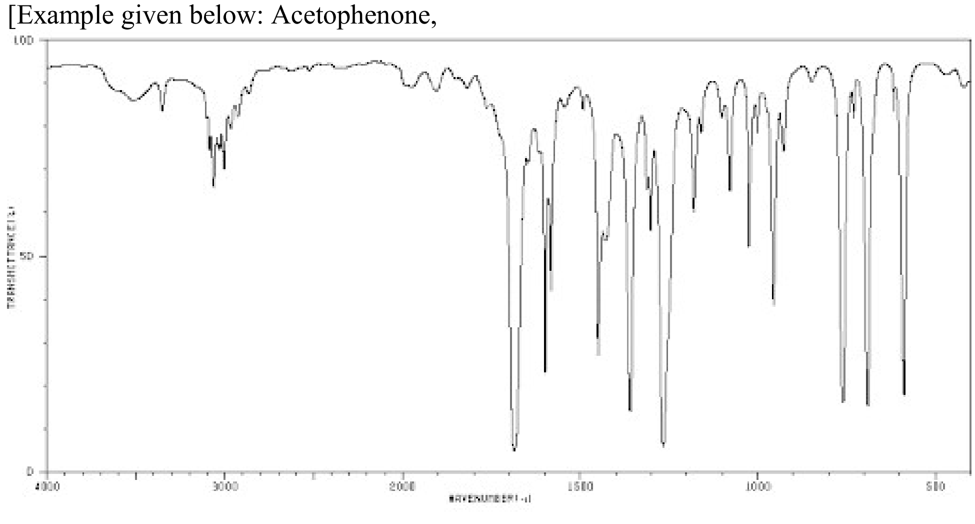
Time: 6 Hrs MSCHE03&04C16 Organic Chemistry Practical II Max. Marks. 40

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