

FAROOK COLLEGE (AUTONOMOUS)

Farook College PO, Kozhikode-673 632

MSc PROGRAMME IN CHEMISTRY

Under Choice Based Credit Semester System

SYLLABUS

Core & Elective Courses

(2022 Admission Onwards)



BOARD OF STUDIES IN CHEMISTRY

CERTIFICATE

I hereby certify that the documents attached are the bonafide copies of the syllabus of Core Courses offered to B.Sc. Chemistry programme and Complementary & Open Courses offered by the Department of Chemistry to be effective from 2022 admission onwards.

Principal

Date:

Place: Farook College

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POSTGRADUATE PROGRAMME IN CHEMISTRY

PREAMBLE

The Master of Science (MSc) in Chemistry is a two-year full-time programme. Science education is central to the development of any society. This can be achieved only by revamping the postgraduate programme to make it effective and meaningful. The development of scientific temper in society necessitates proper education and guidance. In order to achieve this, one must update the developments in the field of science. An effective science education can be imparted at the postgraduate level only by revamping the present curriculum.

To achieve this goal, the curriculum should be restructured by emphasizing various aspects such as the creativity of students, knowledge of current developments in the discipline, awareness of environmental impacts due to the development of science and technology, and the skills essential for handling equipments and instruments in laboratories and industries.

Chemistry, being an experimental science, demands testing theories through practical laboratory experiences for a thorough understanding of the subject. Nowadays, chemistry laboratories in academic institutions use large amounts of chemicals. The awareness and implementation of eco-friendly experiments becomes a global necessity. It is essential to ensure that laboratory chemicals are used at a minimal level without affecting the skill and understanding aimed through laboratory sessions. This creates an environmental awareness among the students and pollution free atmosphere in the campus.

During the preparation of the syllabus, the existing syllabus, the syllabi of undergraduate course and the syllabi of other universities have been referred. Care has been taken to ensure that the syllabus is compatible with the syllabi of other universities at the same level. Sufficient emphasis is given in the syllabus for training in laboratory skills and instrumentation.

The goal of the syllabus is to make the study of chemistry stimulating, relevant and interesting. This curriculum has been prepared with the objective of giving sound knowledge and understanding of chemistry to students with a view to equip them with the potential to contribute to academic, research and industrial environments.

This curriculum will expose students to various fields in chemistry and develop interest in related disciplines. The updated syllabus is based on an interdisciplinary approach to understand the application of the subject in daily life.

The curriculum is designed as per the Regulations of University of Calicut. The revised syllabus is an outcome of several meetings of the board of studies and consultation with various experts in specific subjects from other colleges and universities. Their valuable comments and suggestions have been incorporated in the syllabus. I express my gratitude to members of the board of studies and other experts.

Dr. A. P. Kavitha

Chairperson, Board of Studies in Chemistry (PG)

Farook College (Autonomous)

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AUDIT COURSES

1. Ability Enhancement Course (AEC):

This course aims to have hands on experience for the students in their respective field of study, both in the core and elective subject area. Also, it is a platform for the student community to have basic concepts of research and publication.

AEC is a **4-credit course** and should be conducted during the **first semester** of the programme. Credit of the AE course will not be considered while calculating the SGPA/CGPA. But the student has to obtain minimum pass requirements in this course, which is compulsory for overall pass in the programme

One particular AEC may be selected for all the students in a batch in the department or each student in a batch may choose one AEC, among the pool of courses suggested below. Either a single faculty from the department may be in charge of this course for a batch or each student may be assigned to a particular faculty in the department, in charge of this AEC, which will be decided by the department council/ HoD.

1. Industrial/Research institution visit/visits.
2. Publication of a research article/articles in national/international journal
3. Presentation of research paper/papers in national level seminar/conference, which should be published in the seminar/conference proceedings.
4. Review article/articles on research topics which is presented in a national level seminar/conference and published in the proceedings.
5. Internships at any reputed research institutions/R&D centre/Industry

After conducting the AEC, the evaluation/examination should be done either common for all students in a batch or individually depending upon the AEC conducted. Evaluation/examination must be conducted by **30 weightage** pattern, as in the theory courses. The evaluation/ examination must be conducted jointly by the teacher in charge of the AEC and the head of the department. The result of the AEC, duly signed and sealed by both teacher in charge and head of the department, should be uploaded during the stipulated time period in the third semester of the programme.

Evaluation/examination on AEC must contain the following components:

- a. MCQ type written examination
- b. Report on AEC

- c. Presentation of AEC
- d. Viva voce on AEC.

Distribution of 30 weightage may be done by the teacher in charge in concurrence with the Head of the department.

2. Professional Competency Course (PCC):

This course particularly aims to improve the skill level of students, especially for using specific as well as nonspecific software useful in their respective field of study, both related to the core and elective subject area. Also, it is a platform for the student community to undertake socially committed projects and thereby developing a method of learning process by through the involvement with society.

PCC is a **4-credit course** and should be conducted during the **second semester** of the programme. The credit of the PC course will not be considered while calculating the SGPA/CGPA. But the student has to obtain minimum pass requirements in this course, which is compulsory for an overall pass in the programme.

One particular PCC may be selected for all the students in a batch in the department or each student in a batch may choose one PCC, among the pool of courses suggested below. The exact title of the course may be decided by the department, but the area of study should be from the pool of courses suggested below. Either a single faculty from the department may be in charge of this course for a batch or each student may be assigned to a particular faculty in the department, in charge of this PCC, which will be decided by the department council/ HoD.

1. Development of skills on using softwares like Gaussian, GAMESS etc which is useful in molecular modeling, drug designing, etc.
2. Development of skills on using software like ChemDraw, ChemWindow, ISIS draw, etc which is useful in drawing purposes, structural predictions, etc.
3. Training on computational chemistry
4. Case study and analysis on any relevant issues in the nearby society (e. g. example water analysis, soil analysis, acid/alkali content analysis, sugar content analysis, etc)
5. Any community linking programme relevant to the area of study (e. g. training for society on soap/perfume making, waste disposal, plastic recycling, etc)

After conducting the PCC, the evaluation/examination should be done either common for all students in a batch or individually depending upon the PCC conducted. Evaluation/examination must be conducted by **30 weightage** pattern, as in the theory courses. The evaluation/ examination must be conducted jointly by the teacher in charge of the PCC and the head of the department. The result of the PCC, duly signed and sealed by both teacher in charge and head of the department, should be uploaded during the stipulated time period in the third semester of the programme.

Evaluation/examination on PCC must contain the following components:

- a. MCQ type written examination
- b. Report on PCC
- c. Presentation on PCC
- d. Viva voce on PCC.

Distribution of 30 weightage may be done by the teacher in charge in concurrence with the Head of the department.

PROGRAMME OUTCOME

Upon completion of the postgraduate program at Farook College (Autonomous), the students will be able to develop:

PO1. Advanced Disciplinary Knowledge

Graduates will demonstrate a deep understanding of advanced concepts and theories in their field of study and will be able to apply this knowledge to complex problems.

PO2. Application of knowledge

The graduate will be able to review the information, develop lines of argument and make sound judgment in accordance with the major disciplinary theories and concepts

PO3. Research and Inquiry

Graduates will be able to conduct independent research, using appropriate methods and tools, and will be able to analyse and interpret data to develop evidence-based conclusions

PO4. Professional Practice

Graduates will demonstrate the ability to apply their knowledge and skills to real-world problems and to practice their profession in an ethical and responsible manner.

PO5. Scientific Communication Skills

Students will be able to develop strong scientific communication skills, including the ability to effectively communicate scientific research to both scientific and non-scientific audiences.

PO6. Leadership and Management

Graduates will be able to assume leadership roles, guiding and motivating others to achieve shared goals, and will demonstrate the ability to manage complex projects and teams.

PO7. Lifelong Learning

Graduates will demonstrate a commitment to lifelong learning and professional development, staying current with advances in their field and continuously improving their skills and knowledge.

PROGRAMME SPECIFIC OUTCOMES (PSO)

Upon completion of MSc Chemistry programme, the students will be able to:

- PSO 1. Remember the theoretical and experimental background of different branches of chemistry to understand new concepts.
- PSO 2. Understand the ideas and principle of Inorganic, Organic, Theoretical, and Physical chemistry and interrelate them.
- PSO 3. Analyse and relate the concept acquired with other interdisciplinary areas like biochemistry, computational chemistry, material science, and medicinal chemistry.
- PSO 4. Apply the concepts experimentally by using different equipments to develop practical skills.
- PSO 5. Evaluate the data obtained from computational and experimental measurements.
- PSO 6. Understand the concept through instrumentation and analyse the data obtained for solving the problems.
- PSO 7. Create project report for the research work by using modern analytical methods and instruments.
- PSO 8. Apply the in-depth knowledge of the concepts acquired to qualify competitive examinations.
- PSO 9. Create and invent innovative methods to solve environmental issues.
- PSO 10. Create and design a green protocol for the wellbeing of society by coordinating the ideas obtained from different branches of chemistry.
- PSO 11. Apply the ideas and skills acquired for higher studies in research institutions and to work in chemical industries.

SCHEME OF THE PROGRAMME

Credit and Weightage Distribution in Each Semester

Semester	Course Title	Credits	Weightage		
			Internal	External	
I	Quantum Mechanics and Group Theory	4	30	5	
	Chemistry of Elements	4	30	5	
	Structure and Reactivity of Organic Compounds	4	30	5	
	Thermodynamics, Kinetics and Catalysis	4	30	5	
	<i>Ability Enhancement Course</i>	4	30	-	
	Total credits:	<i>Core Course</i>	16		
		<i>Audit Course</i>	4		
Total		20			
II	Quantum Mechanics and Computational Chemistry	3	30	5	
	Coordination Chemistry	3	30	5	
	Organic Reaction Mechanisms	3	30	5	
	Electrochemistry, Solid State Chemistry and Statistical Thermodynamics	3	30	5	
	Inorganic Chemistry Practical II	3	30	10	
	Organic Chemistry Practical II	3	30	10	
	Physical Chemistry Practical II	3	30	10	
	<i>Professional Competency Course</i>	4	30	-	
	Total credits:	<i>Core Course</i>	21		
<i>Audit Course</i>		4			
Total		25			
III	Molecular Spectroscopy	4	30	5	
	Organometallic & Bioinorganic Chemistry	4	30	5	
	Reagents and Transformations in Organic Chemistry	4	30	5	
	<i>Elective Course-1</i>	4	30	5	
	Total credits:	<i>Core Course</i>	12		
<i>Elective Course</i>		4			
Total		16			

IV	Instrumental Methods of Analysis		4	30	5	
	Inorganic Chemistry Practical IV		3	30	10	
	Organic Chemistry Practical IV		3	30	10	
	Physical Chemistry Practical IV		3	30	10	
	<i>Elective Course-2</i>		4	30	5	
	<i>Elective Course-3</i>		4	30	5	
	Research Project		4	30	5	
	Viva Voce		2	30	5	
	Total credits	<i>Core Course</i>		<i>13</i>		
		<i>Elective Course</i>		<i>8</i>		
<i>Project</i>		<i>4</i>				
<i>Viva Voce</i>		<i>2</i>				
Total		27				
Total credits of the Programme	Core Course		62			
	Elective Course		12			
	Project		4			
	Viva Voce		2			
	Audit Course		8			
	Total Credits		88			

CREDIT DISTRIBUTION

Semester	Core Course	Elective Course	Project	Viva	Audit Course	Total
1	4 + 4 + 4 + 4				4	20
2	3 + 3 + 3 + 3 + 3* + 3* + 3*				4	25
3	4 + 4 + 4	4				16
4	4 + 3* + 3* + 3*	4 + 4	4	2		27
Total	62	12	4	2	8	88

*Practical

COURSE STRUCTURE

Courses offered for M.Sc. Chemistry Programme under CBCSS Pattern

Semester	Course Code	Course Title	Hrs/Week	Credits	Weightage	
					Internal	External
SEMESTER I						
I	MCH1C01	Quantum Mechanics and Group Theory	4	4	30	5
	MCH1C02	Chemistry of Elements	3	4	30	5
	MCH1C03	Structure and Reactivity of Organic Compounds	3	4	30	5
	MCH1C04	Thermodynamics, Kinetics and Catalysis	3	4	30	5
	MCH1L01	Inorganic Chemistry Practical I*	4	-		
	MCH1L02	Organic Chemistry Practical I*	4	-		
	MCH1L03	Physical Chemistry Practical I*	4	-		
	<i>AUD1</i>	<i>Ability Enhancement Course</i>			<i>4</i>	<i>30</i>
	Total credits:	Core Course			16	
Audit Course			4			
Total			20			
SEMESTER II						
II	MCH2C05	Quantum Mechanics and Computational Chemistry	3	3	30	5
	MCH2C06	Coordination Chemistry	3	3	30	5
	MCH2C07	Organic Reaction Mechanisms	3	3	30	5
	MCH2C08	Electrochemistry, Solid State Chemistry and Statistical Thermodynamics	3	3	30	5
	MCH2L04	Inorganic Chemistry Practical II	4	3	30	10
	MCH2L05	Organic Chemistry Practical II	4	3	30	10
	MCH2L06	Physical Chemistry Practical II	4	3	30	10
	<i>AUD2</i>	<i>Professional Competency Course</i>			<i>4</i>	<i>30</i>
	Total credits:	Core Course			21	
Audit Course			4			
Total			25			
SEMESTER III						
III	MCH3C09	Molecular Spectroscopy	4	4	30	5
	MCH3C10	Organometallic & Bioinorganic Chemistry	3	4	30	5
	MCH3C11	Reagents and Transformations in Organic Chemistry	3	4	30	5
	MCH3L07	Inorganic Chemistry Practical III [#]	4			
	MCH3L08	Organic Chemistry Practical III [#]	4			

	MCH3L09	Physical Chemistry Practical III [#]	4			
	MCH3E01	<i>Synthetic Organic Chemistry (Elective)[§]</i>	3	4	30	5
	MCH3E02	Computational Chemistry (Elective) [§]	3	4	30	5
	MCH3E03	Green and Nanochemistry (Elective) [§]	3	4	30	5
	Total Credits:		Core	12		
			Elective [§]	4		
			Total	16		
SEMESTER IV						
IV	MCH4C12	Instrumental Methods of Analysis	4	4	30	5
	MCH4L10	Inorganic Chemistry Practical IV	3	3	30	10
	MCH4L11	Organic Chemistry Practical IV	3	3	30	10
	MCH4L12	Physical Chemistry Practical IV	3	3	30	10
	MCH4E04	Petrochemicals and Cosmetics (Elective) [†]	4	4	30	5
	MCH4E05	Industrial Catalysis (Elective) [†]	4	4	30	5
	MCH4E06	<i>Natural Products & Polymers (Elective)[†]</i>	4	4	30	5
	MCH4E07	Material Science (Elective) [†]	4	4	30	5
	MCH4E08	<i>Organometallic Chemistry (Elective)[†]</i>	4	4	30	5
	MCH4E09	<i>Advanced Topics in Chemistry (Elective)[†]</i>	4	4	30	5
	MCH4P01	Research Project	3	4	30	5
	MCH4V01	Viva Voce		2	30	5
		Total Credits:		Core	13	
	Elective [†]			8		
	Project			4		
	Viva Voce			2		
	Total			27		
Total Credits of the Programme			Core	62		
			Elective	12		
			Project	4		
			Viva Voce	2		
			<i>Audit</i>	<i>8</i>		
			Total Credits	88		

* Exam will be held at the end of 2nd semester

Exam will be held at the end of 4th semester

§ In the third semester, Department can choose any one among the three courses.

† In the fourth semester, Department can choose any two among the six courses.

MSc CHEMISTRY SYLLABUS

SEMESTER I

Theory

MCH1C01 QUANTUM MECHANICS AND GROUP THEORY	1
MCH1C02 CHEMISTRY OF ELEMENTS	9
MCH1C03 STRUCTURE AND REACTIVITY OF ORGANIC COMPOUNDS.....	14
MCH1C04 THERMODYNAMICS, KINETICS AND CATALYSIS	22

SEMESTER II

Theory

MCH2C05 QUANTUM MECHANICS AND COMPUTATIONAL CHEMISTRY.....	28
MCH2C06 COORDINATION CHEMISTRY	34
MCH2C07 REACTION MECHANISM IN ORGANIC CHEMISTRY	40
MCH2C08 ELECTROCHEMISTRY, SOLID STATE CHEMISTRY AND STATISTICAL THERMODYNAMICS.....	47

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MCH1L02 & MCH2L05 ORGANIC CHEMISTRY PRACTICALS– I & II.....	56
MCH1L03 & MCH2L06 PHYSICAL CHEMISTRY – I & II.....	59

SEMESTER III

Theory

MCH3C09 MOLECULAR SPECTROSCOPY.....	63
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MCH3E01 SYNTHETIC ORGANIC CHEMISTRY (ELECTIVE)	82
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MCH3E03 GREEN CHEMISTRY AND NANOCHEMISTRY (ELECTIVE).....	92

SEMESTER IV

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MCH3L09 & MCH4L12 PHYSICAL CHEMISTRY PRACTICALS– III & IV	111
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Elective

MCH4E04 PETROCHEMICALS AND COSMETICS (ELECTIVE).....	116
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MCH4E05 INDUSTRIAL CATALYSIS (ELECTIVE)	122
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MCH4E06 NATURAL PRODUCTS & POLYMER CHEMISTRY (ELECTIVE).....	128
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MCH4E07 MATERIAL SCIENCE (ELECTIVE)	135
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MCH4E08 ORGANOMETALLIC CHEMISTRY (ELECTIVE).....	141
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MCH4E09 ADVANCED TOPICS IN CHEMISTRY (ELECTIVE)	147
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Project

MCH4P01 RESEARCH PROJECT	154
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Viva Voce

MCH4V01 VIVA VOCE.....	156
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LIST OF ELECTIVES

SEMESTER	No.	COURSE CODE & TITLE	Page No.
SEMESTER III	1	MCH3E01 SYNTHETIC ORGANIC CHEMISTRY	82
	2	MCH3E02 COMPUTATIONAL CHEMISTRY	87
	3	MCH3E03 GREEN CHEMISTRY AND NANOCHEMISTRY	92
SEMESTER IV	4	MCH4E04 PETROCHEMICALS AND COSMETICS	116
	5	MCH4E05 INDUSTRIAL CATALYSIS	122
	6	MCH4E06 NATURAL PRODUCTS & POLYMER CHEMISTRY	128
	7	MCH4E07 MATERIAL SCIENCE	135
	8	MCH4E08 ORGANOMETALLIC CHEMISTRY	141
	9	MCH4E09 ADVANCED TOPICS IN CHEMISTRY	147

MSc CHEMISTRY SYLLABUS

Core and Electives

MSc CHEMISTRY SYLLABUS (CBCSS PATTERN)
SEMESTER I

COURSE CODE –MCH1C01				
QUANTUM MECHANICS AND GROUP THEORY				
Credit	Hours/week	Weightage		
		Internal	External	Total
4	4	5	30	35

Course Outcomes

CO No.	Expected Course Outcome	Learning Domain	PSO No
	Upon completion of this course, students will be able to;		
CO1	<i>Understand</i> the laws of quantum mechanics necessary for the description of atoms and molecules and their chemical reaction	Understand	PSO 1
CO2	<i>Distinguish</i> classical and quantum mechanics	Evaluate	PSO 2
CO3	<i>Translate</i> a physical description of quantum mechanics problems	Create	PSO 3
CO4	<i>Achieve</i> physical insight through the mathematics of a problem	Create	PSO 3
CO5	<i>Apply</i> various mathematical equations to different quantum mechanical problems	Apply	PSO 4
CO6	<i>Distinguish</i> various symmetry elements	Analyse	PSO 3
CO7	<i>Find out</i> point group of a molecule and their systematic identification	Analyse	PSO 3
CO8	Construct group multiplication tables	Create	PSO 3
CO9	Judge the suitability of group theoretical methods for spectroscopy.	Evaluate	PSO 3
CO10	Evaluate the suitability of group theoretical methods for solving chemical bonding.	Evaluate	PSO 10

COURSE CONTENT

Unit 1: Mathematics for Chemists	5 Hours
<p>1.1. Matrix Algebra: Addition and multiplication, inverse, adjoint and transpose of matrices, special metrics (symmetric, skew –symmetric, Hermitian, skew-Hermitian, unit diagonal, unitary etc) and their properties. block factored matrices, Matrix equations: Homogenous, non-homogenous linear equations and conditions for the solution, linear dependence and independence.</p> <p>1.2. Differential calculus: Functions, continuity and differentiability, rules for differentiation, application of differential calculus including maxima and minima, Functions of various variables, partial differentiation.</p> <p>1.3. Integral calculus: Basic rules for integration, integration by parts, partial fraction and substitution, Reduction formulae, applications of integral calculus.</p> <p>1.4. Coordinate Systems: Cartesian, and spherical polar coordinates and their relationships</p> <p>1.5. Complex Numbers: Algebraic operations, modulus and conjugate</p>	
Unit 2: Introduction to Quantum Mechanics	8 Hours
<p>2.1. Black body radiation and Planck’s quantum postulate. Einstein’s photoelectric equation, Schrodinger’s wave mechanics,</p> <p>2.2. Detailed discussion of postulates of quantum mechanics – State function or wave function postulate, Born interpretation of the wave function, well behaved functions, orthonormality of wave functions</p> <p>2.3. Operator postulate, operator algebra, linear and nonlinear operators, Non-commuting operators and the Heisenberg’s Uncertainty principle, Laplacian operator, Hermitian operators and their properties, eigen functions and eigen values of an operator</p> <p>2.4. Eigen value postulate, eigen value equation, Expectation value postulate;</p> <p>2.5. Postulate of time- dependent Schrödinger equation of motion, conservative systems and time independent Schrödinger equation. Stationary states.</p>	

Unit 3: Quantum Mechanics of Translational & Vibrational Motions	8 Hours
<p>3.1. Free particle in one-dimension; Particle in a one-dimensional box with infinite potential walls, important features of the problem; Particle in a one-dimensional box with one finite potential wall, Particle in a rectangular well, (no derivation), Significance of the problem,</p> <p>3.2. Introduction to tunnelling</p> <p>3.3. Particle in a three-dimensional box, Separation of variables, degeneracy, Symmetry breaking.</p> <p>3.4. One-dimensional harmonic oscillator (complete treatment):- Method of power series, Hermite equation and Hermite polynomials, recursion relation, wave functions and energies, important features of the problem</p> <p>3.5. Harmonic oscillator model and molecular vibrations.</p>	
Unit 4: Quantum Mechanics of Rotational Motion	8 Hours
<p>4.1. Planar rigid rotor (or particle on a ring), the Phi-equation, solution of the Phi-equation</p> <p>4.2. One particle Rigid rotator (non-planar rigid rotator or particle on a sphere) (complete treatment): The wave equation in spherical polar coordinates, separation of variables, the Phi-equation and the Theta-equation and their solutions, Legendre and associated Legendre equations, Legendre and associated Legendre polynomials, Rodrigue's formula, spherical harmonics (imaginary and real forms), polar diagrams of spherical harmonics.</p> <p>4.3. Quantization of angular momentum, quantum mechanical operators corresponding to angular momenta (L_x, L_y, L_z), commutation relations between these operators, Ladder operator method for angular momentum, space quantization.</p>	
Unit 5: Quantum Mechanics of Hydrogen-like Atoms	8 Hours
<p>5.1. Potential energy of hydrogen-like systems, the wave equation in spherical polar coordinates, separation of variables, the R, Theta and Phi equations and their solutions, Laguerre and associated Laguerre polynomials, wave functions</p>	

<p>and energies of hydrogen-like atoms, orbitals, radial functions and radial distribution functions and their plots, angular functions (spherical harmonics) and their plots.</p> <p>5.2. The postulate of spin by Uhlenbeck and Goudsmith, Dirac's relativistic equation for hydrogen atom and discovery of spin (qualitative treatment),</p> <p>5.3. Spin orbitals, construction of spin orbitals from orbitals and spin functions.</p>	
<p>Unit 6: Basic principles of group theory and Representation of Point groups</p>	<p>11 Hours</p>
<p>6.1. Introduction - the defining properties of mathematical groups, finite and infinite groups, Abelian and cyclic groups, group multiplication tables (GMT), similarity transformation, sub groups & classes in a group.</p> <p>6.2. Molecular Symmetry & point groups - symmetry elements and symmetry operations in molecules, relations between symmetry operations, complete set of symmetry operations of a molecule, point groups and their systematic identification, GMT of point groups</p> <p>6.3. Representations of point groups - basis for a representation, representations using vectors, atomic orbitals and Cartesian coordinates positioned on the atoms of molecule (H₂O as example) as bases, reducible representations and irreducible representations (IR) of point groups, construction of IR by reduction (qualitative demonstration only)</p> <p>6.4. Great Orthogonality Theorem (GOT) (no derivation) and its consequences, derivation of characters of IR using GOT, construction of character tables of point groups (C_{2v}, C_{3v}, C_{2h} and C_{4v} and C₃ as examples), nomenclature of IR - Mulliken symbols, symmetry species; Reduction formula - derivation of reduction formula using GOT, reduction of reducible representations, (e.g., G_{cart}) using the reduction formula.</p> <p>6.5. Relation between group theory and quantum mechanics – wavefunctions (orbitals) as bases for IR of point groups.</p>	
<p>Unit 7: Applications of Group Theory to Molecular Spectroscopy</p>	<p>8 Hours</p>

<p>7.1. Molecular vibrations - symmetry species of normal modes of vibration, construction of G_{cart}, normal coordinates and drawings of normal modes (e.g., H_2O and NH_3), selection rules for IR and Raman activities based on symmetry arguments, determination of IR active and Raman active modes of molecules (e.g., H_2O, NH_3, CH_4, SF_6), complementary character of IR and Raman spectra.</p> <p>7.2. Spectral transition probabilities - direct product of irreducible representations and its use in identifying vanishing and non-vanishing integrals, transition moment integral and spectral transition probabilities.</p> <p>7.3. Electronic Spectra – electronic transitions and selection rules, Laporte selection rule for Centro symmetric molecules.</p>	
<p>Unit 8: Applications of Group Theory to Chemical Bonding</p>	<p>8 Hours</p>
<p>8.1. Hybridisation - Treatment of hybridization in BF_3 and CH_4,</p> <p>8.2. Inverse transformation and construction of hybrid orbitals. Molecular orbital theory – $HCHO$ and H_2O as examples,</p> <p>8.3. Classification of atomic orbitals involved into symmetry species, group orbitals, symmetry adapted linear combinations (SALC), projection operator,</p> <p>8.4. Construction of SALC using projection operator, use of projection operator in constructing SALCs for the pMOs in cyclopropenyl ($C_3H_3^+$) cation.</p>	

<p>MODE OF TRANSACTION</p>
<p>Face to Face Instruction: This involves attending traditional classroom lectures and participating in in-person discussions and activities with the instructor and fellow students.</p> <p>Peer to Peer learning: Students have to select a topic in the course and present it in the class which providing opportunity for critical thinking and feedback.</p> <p>Group Discussion: Group discussion will be conducted based on the relevant topic in the course that will improve students' thinking and help them to construct their own meaning about academic contents.</p>

MODE OF ASSESSMENT					
Internal Assessment (15 Weightage)					
a. Internal Examination		2 Weightage			
<i>2 Internal Examinations, both should be considered</i>					
b. Assignments and Exercises:		3 Weightage			
c. Seminar/ Viva Voce:		3 Weightage			
d. Attendance:		3 Weightage			
External Assessment (30 Weightages) Duration 3 Hours, No of Questions: 23					
PATTERN OF QUESTION PAPER					
Division	Type	Total No. of questions	No. of questions to be answered	Weightages for each question	Total Weightage
Section A	Short	12	8	1	8
Section B	Short Essay	7	4	3	12
Section C	Essay	4	2	5	10
Total					30

MODULE WISE WEIGHTAGE DISTRIBUTION	
Module	Mark
Unit 1: Mathematics for Chemists	3
Unit 2: Introduction to Quantum Mechanics	6
Unit 3: Quantum Mechanics of Translational & Vibrational Motions	6
Unit 4: Quantum Mechanics of Rotational Motion	6
Unit 5: Quantum Mechanics of Hydrogen-like Atoms	6

Unit 6: Basic principles of group theory and Representation of Point	8
Unit 7: Applications of Group Theory to Molecular Spectroscopy	6
Unit 8: Applications of Group Theory to Chemical Bonding	5

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M.Sc. CHEMISTRY (CBCSS PATTERN)
SEMESTER I

COURSE CODE –MCH1C02				
CHEMISTRY OF ELEMENTS				
Credit	Hours/week	Weightage		
		Internal	External	Total
4	3	5	30	35

Course Outcomes

CO No.	Expected Course Outcome	Learning Domain	PSO No
	Upon completion of this course, students will be able to;		
CO1	Identify acids and bases based on different acid-base concepts.	Remember	PSO 1
CO2	Compare acid and base strengths	Evaluate	PSO 3
CO3	Summarize the chemistry of main group elements	Understand	PSO 8
CO4	Construct diagrams of reduction potentials	Create	PSO 3
CO5	Illustrate various concepts of atomic nucleus	Analyse	PSO 2
CO6	Classify different polyhedral structure.	Understand	PSO 1
CO7	Distinguish reactions in different types of solvents	Analyse	PSO 3
CO8	Judge choice of suitable solvent for reactions.	Evaluate	PSO 10
CO9	Differentiate magnetic properties of substances.	Analyze	PSO 6

COURSE CONTENT

Unit 1: Concepts of Acids and Bases, and Nonaqueous Solvents	8 hours
<p>1.1. Major acid-base concepts, Arrhenius, Bronsted-Lowry, Solvent system, Lux-Flood, Lewis and Usanovich concepts. HSAB principle.-Theoretical basis of hardness and softness.</p> <p>1.2. The Drago-Wayland equation, E and C parameters- Symbiosis.</p> <p>1.3. Applications of HSAB concept.</p> <p>1.4. Super acids, superbases, surface acidity.</p> <p>1.5. Chemistry of nonaqueous solvents- NH₃, SO₂, H₂SO₄, BrF₃, HF, N₂O₄ and HSO₃F. Nonaqueous solvents and acid-base strength.</p>	
Unit 2: Chemistry of Main Group Elements-I	8 hours
<p>2.1. Boron hydrides-preparation, reactions, structure, and bonding.</p> <p>2.2. Styx numbers-closo, nido, arachno polyhedral structures.</p> <p>2.3. Boron cluster compounds-Wade's rule.</p> <p>2.4. Polyhedral borane anion-carboranes, metallaboranes and metallacarboranes.</p> <p>2.5. Borazines and borides.</p>	
Unit 3: Chemistry of Main Group Elements-II	8 hours
<p>3.1. Silicates and alumino silicates-Structure, molecular sieves-Zeolite.</p> <p>3.2. Silicones-Synthesis, structure and uses. Carbides and silicides.</p> <p>3.3. Synthesis, structure, bonding and uses of Phosphorous-Nitrogen, Phosphorous-Sulphur and Sulphur-Nitrogen compounds.</p>	
Unit 4: Standard reduction potentials and their diagrammatic representations	8 hours
<p>4.1. Ellingham diagram. Latimer and Frost diagrams. Pourbaix diagram.</p> <p>4.2. Heteropoly and isopoly anions of V, Cr, W, Mo, Polyatomic Zintl anions and cations.</p> <p>4.3. Chevrel phases.</p>	
Unit 5: Magnetic properties of Transition Inner Transition Elements	8 hours

<p>5.1. Term symbols. Magnetic property - Paramagnetism, Diamagnetism, Ferromagnetism, Antiferromagnetism, Ferrimagnetism.</p> <p>5.2. Magnetic susceptibility. Curie and Curie-Weiss Law.</p> <p>5.3. Magnetic moment and its expressions. Quenching of orbital magnetic moment. Magnetic exchange interactions-Superexchange and direct exchange.</p> <p>5.4. Determination of magnetic moment of complexes -Gouy Method, Faraday Method, VSM and SQUID.</p> <p>5.5. Uranyl compounds. Trans-actinide elements.</p>	
<p>Unit 6: Nuclear and Radiation Chemistry</p>	<p>8 hours</p>
<p>6.1. Structure of nucleus: shell, liquid drop, Fermi gas, collective and optical models.</p> <p>6.2. Nuclear reaction: Bethe's notation of nuclear process- Types-reaction cross section- photonuclear and thermonuclear reactions. Super heavy elements – production and chemistry.</p> <p>6.3. Nuclear fission: Theory of fission- neutron capture cross section and critical size. Nuclear fusion. Neutron activation analysis</p> <p>6.4. Radiation chemistry: Interaction of radiation with matter. Detection and measurement of radiation- GM and scintillation counters – radiolysis of water - radiation hazards - radiation dosimetry.</p>	

<p>MODE OF TRANSACTION</p>
<p>Face to Face Instruction: This involves attending traditional classroom lectures and participating in in-person discussions and activities with the instructor and fellow students.</p> <p>Peer to Peer learning: Students have to select a topic in the course and present it in the class which providing opportunity for critical thinking and feedback.</p>

Unit 5: Magnetic properties of Transition Inner Transition Elements	8
Unit 6: Nuclear and Radiation Chemistry	7

REFERENCES:

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2. J.E. Huheey, E.A. Keiter, R.L. Keiter. O.K. Medhi. Inorganic Chemistry, principles of structure and reactivity, Pearson Education, 2006.
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M.Sc. CHEMISTRY (CBCSS PATTERN)
SEMESTER I

COURSE CODE –MCH1C03				
STRUCTURE AND REACTIVITY OF ORGANIC COMPOUNDS				
Credit	Hours/week	Weightage		
		Internal	External	Total
4	3	5	30	35

Course Outcomes

CO No.	Expected Course Outcome	Learning Domain	PSO No
	Upon completion of this course, students will be able to;		
CO1	Explain and discuss the structure, stability and bonding in organic molecules.	Understand	PSO 2
CO2	Compare and justify the impact of molecular structure on reactivity of different types of organic reactions.	Evaluate	PSO 3
CO3	Explain and design methods from the idea of molecular conformation, mechanism and stereochemical outcome.	Create	PSO 10
CO4	Examine and interpret the different methods of asymmetric synthesis for synthetic applications	Apply	PSO 8
CO5	Apply the concept of stereochemistry to different organic compounds and reactions	Apply	PSO 4
CO6	Distinguish and develop suitable mechanism using stereochemical aspects.	Analyse	PSO 3
CO7	Illustrate various concepts of organic mechanism relating with stereochemistry	Apply	PSO 10

COURSE CONTENT

Unit 1: Structure and Bonding in Organic Molecules	8 Hours
<p>1.1. Nature of Bonding in Organic Molecules: Localized and delocalized chemical bonding, bonding weaker than covalent bond, cross- conjugation, resonance, rules of resonance, resonance hybrid and resonance energy, tautomerism, hyperconjugation, π-π interactions, $p\pi$-$d\pi$ bonding (ylides).</p> <p>1.2. Stability of benzylic cations and radicals. Effect of delocalized electrons on pKa.</p> <p>1.3. Hydrogen bonding: Inter and intra-molecular hydrogen bonding. Range of the energy of hydrogen bonding.</p> <p>1.4. Physical and chemical properties of organic compounds- volatility, acidity, basicity and stability, stabilization of hydrates of glyoxal, chloral, and ninhydrin, high acid strength of maleic acid compared to fumaric acid. Effect of hydrogen bond on conformation.</p> <p>1.5. Electron donor-acceptor complexes, crown ether complexes, cryptates, inclusion compounds and cyclodextrins.</p> <p>1.6. Hückel MO method. MO's of simple molecules, ethylene, allyl radical and 1,3-butadiene. Hückel rule and modern theory of aromaticity, criteria for aromaticity and antiaromaticity, MO description of aromaticity and antiaromaticity.</p> <p>1.7. Homoaromaticity. Aromaticity of annulenes and heteroannulenes, fused ring systems, fulvenes, fulvalenes, azulenes, pentalenes and heptalenes.</p>	
Unit 2: Structure and Reactivity	8 Hours
<p>2.1. Transition state theory, Potential energy vs reaction co-ordinate curve, substituent effects (inductive, mesomeric, inductomeric, electomeric and field effects) on reactivity.</p> <p>2.2. Qualitative study of substitution effects in S_N1-S_N2 reactions. Neighbouring group participation, participation of carboxylate ion, halogen, hydroxyl group, acetoxy group, phenyl group and pi -bond. Classical and nonclassical carbocations</p>	

<p>2.3. Basic concepts in the study of organic reaction mechanisms: Application of experimental criteria to mechanistic studies, kinetic versus thermodynamic control- Hammond postulate, Bell-Evans-Polanyi principle, Marcus equation, Curtin-Hammet principles, Acidity constant, Hammett acidity function.</p> <p>2.4. Isotope effect (labelling experiments), stereochemical correlations.</p> <p>2.5. Semiquantitative study of substituent effects on the acidity of carboxylic acids.</p> <p>2.6. Quantitative correlation of substituent effects on reactivity.</p> <p>2.7. Linear free energy relationships. Hammett and Taft equation for polar effects and Taft's steric substituent constant for steric effect. Solvent effects- Dimroth parameter</p>	
<p>Unit 3: Conformational Analysis – I</p>	<p>8 Hours</p>
<p>3.1. Factors affecting the conformational stability of molecules – dipole interaction, bond opposition strain, bond angle strain. Conformation of acyclic compounds – Ethane, n- butane, Influence of dipole moment and hydrogen bonding on conformational stability- Conformation of alkene dihalides, glycols, chlorohydrins, tartaric acid, erythro and threo isomer.</p> <p>3.2. Interconversion of axial and equatorial bonds in chair conformation of cyclohexane– distance between the various H atoms and C atoms in chair and boat conformations.</p> <p>3.3. Monosubstituted cyclohexane–methyl and t-butyl cyclohexanes–flexible and rigid systems. Conformation of 1,2-, 1,3-, and 1,4 disubstituted cyclohexane</p> <p>3.4. Conformation of substituted cyclohexanone, 2-bromocyclohexanone, dibromocyclohexanone, (cis & trans), 2-bromo-4,4-dimethyl cyclohexanone. Anchoring group and conformationally biased molecules.</p> <p>3.5. Conformations of 1,4 -cis and -trans disubstituted cyclohexanes in which one of the substituent is 1-butyl and their importance in assessing the reactivity of an axial or equatorial substituent.</p> <p>3.6. Conformation of 1,2-, 1,3-, and 1,4-cyclohexane diol.</p>	
<p>Unit 4: Conformational Analysis – II</p>	<p>8 Hours</p>

- 4.1. Effect of conformation on the course and rate of reactions in (a) debromination of dl and meso 2,3-dibromobutane or stilbene dibromide using KI. (b) semipinacolic deamination of erythro and threo 1,2-diphenyl-1-(p-chlorophenyl)-2-amino ethanol. (c) dehydro halogenation of stilbene dihalide (dl and meso) and erythro threo- bromo-1,2-diphenyl propane.
- 4.2. Effect of conformation on the course and rate of reactions in cyclohexane systems illustrated by: (a) S_N2 and S_N1 reactions for (i) an axial substituent, and (ii) an equatorial substituent in flexible and rigid systems. (b) E1, E2 eliminations illustrated by the following compounds. (i) 4-t-Butylcyclohexyl tosylate (cis and trans) (ii) 2- Phenylcyclohexanol (cis and trans) (iii) Menthyl and neomenthyl chlorides and benzene hexachlorides. (c) Pyrolytic elimination of esters (cis elimination) (d) Esterification of axial as well as equatorial hydroxyl and hydrolysis of their esters in rigid and flexible systems. (Compare the rate of esterification of methanol, isomenthol, neomenthol and neoisomenthol). (f) Esterification of axial as well as equatorial carboxyl groups and hydrolysis of their esters. (g) Hydrolysis of axial and equatorial tosylates. (h) Oxidation of axial and equatorial hydroxyl group to ketones by chromic acid.
- 4.3. Bredt's rule. Stereochemistry of fused, bridged and caged ring systems- decalins, norbornane, barrelene and adamantanes.

Unit 5: Stereochemistry

8 Hours

- 5.1. Conformation and configuration, Fischer, Newman and Sawhorse projection formulae and their interconversion. Concept of chirality, recognition of symmetry elements and chiral structures, conditions for optical activity, optical purity. Specific rotation and its variation in sign and magnitude under different conditions, relative and absolute configurations, Fisher projection formula, sequence rule – R and S notation in cyclic and acyclic compounds, Cahn-Ingold-Prelog (CIP) rule. Mixtures of stereoisomers; enantiomeric excess and diastereomeric excess and their determination. Methods of resolution diastereomers. Resolution of racemates after conversion into diastereomers; use of S- brucine, kinetic resolution of enantiomers, chiral chromatography.

<p>5.2. Optical isomerism of compounds containing one or more asymmetric carbon atoms, enantiotopic, homotopic, diastereotopic hydrogen atoms, prochiral centre. Pro-R, Pro-S, Re and Si.</p> <p>5.3. Optical isomerism in biphenyls, allenes and nitrogen and sulphur compounds, conditions for optical activity, R and S notations. Optical activity in cis-trans conformational isomers of 1,2-, 1,3- and 1,4-dimethylcyclohexanes.</p> <p>5.4. Restricted rotation in biphenyls – Molecular overcrowding. Chirality due to folding of helical structures. P/M notations, Chirality due to chiral plane-R/S notation</p> <p>5.5. Geometrical isomerism – E and Z notation of compounds with one and more double bonds in acyclic systems. Configuration of cyclic compounds- monocyclic, fused and bridged ring systems, inter conversion of geometrical isomers. Methods of determination of the configuration of geometrical isomers in acyclic and cyclic systems, stereochemistry of aldoximes and ketoximes IUPAC nomenclature of regio and stereo isomers of organic molecules.</p> <p>5.6. stereoselectivity and stereospecificity, enantio selectivity and diastereoselectivity. Stereoselective and stereospecific reactions: (i) Bromination of E- and Z-2-butene-a stereospecific anti addition, (ii) Epoxidation of E- and Z-2 butene-a stereospecific reaction, (iii) Bromination of cyclohexene- a stereoselective reaction, (iv) Hydroboration-Oxidation hydration of alkenes- a stereospecific anti-markovnikov hydration (v) Addition of carbenes to alkenes.</p>	
<p>Unit 6: Asymmetric Synthesis</p>	<p>8 Hours</p>
<p>6.1. Asymmetric synthesis, need for asymmetric synthesis, stereoselectivity and stereospecificity. Chiral pool: chiral pool synthesis of beetle pheromone component (S)- (-)-ipsenol from (S)-(-)-leucine. conversion of L-tyrosine into L-Dopa.</p> <p>6.2. Classification of Asymmetric reactions into (1) Substrate controlled (2) Chiral auxiliary controlled (3) Chiral reagent controlled and (4) Chiral catalyst controlled.</p>	

- 6.3. Substrate controlled asymmetric synthesis: Nucleophilic addition to chiral carbonyl compounds. 1,2-asymmetric induction, Cram's rule and Felkin-Anh model.
- 6.4. Chiral auxiliary controlled asymmetric synthesis: α -Alkylation of chiral enolates, azaenolates, imines and hydrazones, chiral sulfoxides. 1,4-Asymmetric induction and Prelog's rule. Use of chiral auxiliary in Diels-Alder reactions.
- 6.5. Diastereoselective aldol reaction and its explanation by Zimmermann-Traxler model. Auxiliary controlled aldol reaction. Double diastereoselection-matched and mismatched aldol reactions
- 6.6. Chiral reagent controlled asymmetric synthesis: Asymmetric reduction using BINAL-H. Asymmetric hydroboration using IPC2BH and IPCBH2. Reduction with CBH reagent. Stereochemistry of Sharpless asymmetric epoxidation and dihydroxylation. Asymmetric aldol reaction:
- 6.7. Chiral catalyst controlled: Ruthenium catalyst with chiral phosphine, Reduction with CBS reagent, Sharpless asymmetric epoxidation and dihydroxylation.

MODE OF TRANSACTION

Face to Face Instruction: This involves attending traditional classroom lectures and participating in in-person discussions and activities with the instructor and fellow students.

Peer to Peer learning: Students have to select a topic in the course and present it in the class which providing opportunity for critical thinking and feedback.

Group Discussion: Group discussion will be conducted based on the relevant topic in the course that will improve students' thinking and help them to construct their own meaning about academic contents.

MODE OF ASSESSMENT

Internal Assessment (15 Weightage)					
a. Internal Examination		2 Weightage			
<i>2 Internal Examinations, both should be considered</i>					
b. Assignments and Exercises:		3 Weightage			
c. Seminar/ Viva Voce:		3 Weightage			
d. Attendance:		3 Weightage			
External Assessment (30 Weightages) <i>Duration 3 Hours, No of Questions: 23</i>					
PATTERN OF QUESTION PAPER					
Division	Type	Total No. of questions	No. of questions to be answered	Weightages for each question	Total Weightage
Section A	Short	12	8	1	8
Section B	Short Essay	7	4	3	12
Section C	Essay	4	2	5	10
Total					30

MODULE WISE WEIGHTAGE DISTRIBUTION	
Module	Mark
Unit 1: Structure and Bonding in Organic Molecules	7
Unit 2: Structure and Reactivity	8
Unit 3: Conformational Analysis – I	8
Unit 4: Conformational Analysis – II	8
Unit 5: Stereochemistry	8
Unit 6: Asymmetric Synthesis	7

REFERENCES:

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2. M. B. Smith, J. March, March's Advanced Organic Chemistry, John Wiley & Sons, 6/e, 2007.
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M.Sc. CHEMISTRY (CBCSS PATTERN)
SEMESTER I

COURSE CODE – MCH1C04				
THERMODYNAMICS, KINETICS AND CATALYSIS				
Credit	Hours/week	Weightage		
		Internal	External	Total
4	3	5	30	35

Course Outcomes

CO. No	Expected Course Outcome	Learning Domain	PSO No
	Upon completion of this course, students will be able to;		
CO1	<i>Understand</i> laws and concepts in thermodynamics	Remember	PSO 1
CO2	<i>Apply</i> laws and concepts in thermodynamics to solve problems	Apply	PSO8
CO3	<i>Understand</i> various approximations and mechanisms needed to explain kinetics of fast reactions, chain reactions and those involving reactive atoms and free radicals	Remember	PSO 2
CO4	<i>Identify</i> basics of various theories in Chemical Kinetics	Analyse	PSO3
CO5	<i>Apply</i> various theories in Chemical Kinetics to solve problems in kinetics	Apply	PSO8
CO6	<i>Understand</i> fundamental theories and methods in surface chemistry	Remember	PSO 1
CO7	<i>Solve</i> problems in surface chemistry	Apply	PSO8
CO8	<i>Acquire</i> knowledge regarding various mechanisms of catalyzed reactions	Remember	PSO 2
CO9	<i>Recognize</i> various techniques used for surface analyses	Remember	PSO11

COURSE CONTENT

Unit 1: Thermodynamics	8 Hours
<p>1.1. Review of First and Second law of thermodynamics, Third law of thermodynamics, Need for third law, Nernst heat theorem, Apparent exceptions to third law, Applications of Third law, Determination of Absolute entropies, Residual entropy.</p> <p>1.2. Thermodynamics of Solutions: Partial molar quantities, Chemical potential, Variation of chemical potential with temperature and pressure, Partial molar volume and its determination, Gibbs-Duhem equation.</p> <p>1.3. Thermodynamics of ideal and real gases and gaseous mixtures, Fugacities of gases and their determinations, Activity, Activity coefficient, standard state of substance (for solute and solvents)</p> <p>1.4. Duhem-Margules equation and its applications. Thermodynamics of ideal solutions, Deduction of the laws of Raoult's ebullioscopy, cryoscopy, and osmotic pressure.</p> <p>1.5. Non ideal solutions, Deviations from Raoult's law, Excess functions- excess free energy, excess entropy, excess enthalpy, excess volume.</p>	
Unit 2: Thermodynamics of Irreversible Processes	8 Hours
<p>2.1. Thermodynamics of irreversible process: Stationary state concept. Principle of local equilibrium.</p> <p>2.2. Simple examples of irreversible processes, general theory of non-equilibrium processes, forces and fluxes, entropy production in simple irreversible systems (closed systems) involving heat flow only and both heat flow and matter flow,</p> <p>2.3. The phenomenological relations, Onsager relations: Linear relations-coupled flows.</p> <p>2.4. Onsager reciprocal relations (no derivation), application to the theory of diffusion, thermal diffusion, thermo-osmosis and thermo- molecular pressure difference, electro-kinetic effects, the Glansdorf Pregogine equation.</p>	
Unit 3: Chemical Kinetics	8 Hours

<p>3.1. Kinetics of reactions involving reactive atoms and free radicals - Rice - Herzfeld mechanism and steady state approximation in the kinetics of organic gas phase decompositions (acetaldehyde & ethane)</p> <p>3.2. Kinetics of chain reactions – branching chain and explosion limits (H₂-O₂ reaction as an example)</p> <p>3.3. Kinetics of fast reactions- relaxation methods, molecular beams, flash photolysis; Solution kinetics:</p> <p>3.4. Factors affecting reaction rates in solution, Effect of solvent and ionic strength (primary salt effect) on the rate constant, secondary salt effects.</p>	
<p>Unit 4: Molecular Reaction Dynamics</p>	<p>8 Hours</p>
<p>4.1. Reactive encounters: Collision theory, diffusion controlled reactions, the material balance equation, Activated Complex theory – the Eyring equation, thermodynamic aspects of ACT; Comparison of collision and activated complex theories</p> <p>4.2. The dynamics of molecular collisions – Molecular beams, principle of crossed-molecular beams; Potential energy surfaces - attractive and repulsive surfaces, London equation, Statistical distribution of molecular energies</p> <p>4.3. Theories of unimolecular reactions - Lindemann's theory, Hinshelwood's modification, Rice -Ramsperger and Kassel (RRK) model.</p>	
<p>Unit 5: Surface Chemistry</p>	<p>8 Hours</p>
<p>5.1. Structure and chemical nature of surfaces, Adsorption at surfaces - Adsorption isotherms, Langmuir's unimolecular theory of adsorption, BET equation, derivation</p> <p>5.2. Determination of surface area and pore structure of adsorbents - physical adsorption methods, X-ray methods, mercury intrusion method, chemisorption methods.</p> <p>5.3. Determination of surface acidity - TPD method. Heat of adsorption and its determination.</p>	
<p>Unit 6: Catalysis</p>	<p>8 Hours</p>

- 6.1. Features of homogeneous catalysis – Enzyme catalysis - Michaelis-Menten Mechanism.
- 6.2. Features of heterogeneous catalysis - Langmuir-Hinshelwood mechanism and Eley-Rideal mechanism – illustration using the reaction $2\text{CO} + \text{O}_2 \rightarrow 2\text{CO}_2$.
- 6.3. Methods of preparation of heterogeneous catalysts - precipitation and co-precipitation methods, sol gel method, flame hydrolysis.
- 6.4. Preparation of Zeolites and silica supports.
- 6.5. Auto catalysis - oscillating reactions – mechanisms of oscillating reactions (Lotko -Volterra, brusselator and oregonator).

MODE OF TRANSACTION

Face to Face Instruction: This involves attending traditional classroom lectures and participating in in-person discussions and activities with the instructor and fellow students.

Peer to Peer learning: Students have to select a topic in the course and present it in the class which providing opportunity for critical thinking and feedback.

Group Discussion: Group discussion will be conducted based on the relevant topic in the course that will improve students' thinking and help them to construct their own meaning about academic contents.

MODE OF ASSESSMENT

Internal Assessment (15 Weightage)

- | | |
|---|-------------|
| a. Internal Examination | 2 Weightage |
| <i>2 Internal Examinations, both should be considered</i> | |
| b. Assignments and Exercises: | 3 Weightage |
| c. Seminar/ Viva Voce: | 3 Weightage |
| d. Attendance: | 3 Weightage |

External Assessment (30 Weightages) *Duration 3 Hours, No of Questions: 23*

PATTERN OF QUESTION PAPER					
Division	Type	Total No. of questions	No. of questions to be answered	Weightages for each question	Total Weightage
Section A	Short	12	8	1	8
Section B	Short Essay	7	4	3	12
Section C	Essay	4	2	5	10
Total					30

MODULE WISE WEIGHTAGE DISTRIBUTION	
Module	Mark
Unit 1: Thermodynamics	7
Unit 2: Thermodynamics of Irreversible Processes	8
Unit 3: Chemical Kinetics	8
Unit 4: Molecular Reaction Dynamics	8
Unit 5: Surface Chemistry	8
Unit 6: Catalysis	7

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M.Sc. CHEMISTRY (CBCSS PATTERN)
SEMESTER II

COURSE CODE –MCH2C05				
QUANTUM MECHANICS AND COMPUTATIONAL CHEMISTRY				
Credit	Hours/week	Weightage		
		Internal	External	Total
3	3	5	30	35

Course Outcomes

CO No.	Expected Course Outcome	Learning Domain	PSO No
	Upon completion of this course, students will be able to;		
CO1	Develop working knowledge of terminology and tools used by quantum chemists.	Understand	PSO 2
CO2	Evaluate how quantum mechanics manifests itself in nature and experimental science	Evaluate	PSO 3
CO3	Summarize various theories of chemical bonding	Understand	PSO 8
CO4	Construct molecular energy level diagrams	Create	PSO 3
CO5	Correlate Huckel parameters to various descriptors of conjugated systems	Apply	PSO 4
CO6	Learn how computational chemistry can be a valid alternatives and complements to the experimental methods in chemistry.	Understand	PSO 2
CO7	Construct Z matrix of various molecules	Create	PSO 3
CO8	Evaluate choice of suitable computational methods.	Evaluate	PSO 10

COURSE CONTENT

Unit 1: Approximation Methods in Quantum Mechanics	8 Hours
<p>1.1. Many body problem and the need of approximation methods; Independent particle model</p> <p>1.2. Variation method – variation theorem with proof, illustration of variation theorem using a trial function [e.g., $x(a-x)$] for particle in a 1D-box, variation treatment for the ground state of helium atom.</p> <p>1.3. Perturbation method – time-independent perturbation method (non-degenerate case only), illustration by application to particle in a 1D-box with slanted bottom, perturbation treatment of the ground state of the helium atom.</p>	
Unit 2: Quantum Mechanics of Many-electron Atoms	8 Hours
<p>2.1. Hartree’s Self-Consistent Field method for atoms, Fock modification using spin orbitals & Hartree -Fock Self-Consistent Field (HF-SCF) method for atoms, the Fock operator.</p> <p>2.2. Pauli’s antisymmetry principle</p> <p>2.3. Slater determinants; Roothan’s concept of basis functions</p> <p>2.4. Slater type orbitals (STO) and Gaussian type orbitals(GTO).</p>	
Unit 3: Chemical Bonding in Diatomic Molecule	8 Hours
<p>3.1. Schrödinger equation for a molecule, Born – Oppenheimer approximation</p> <p>3.2. Valence Bond (VB) theory – VB theory of H_2 molecule, singlet and triplet state functions (spin orbitals) of H_2.</p> <p>3.3. Molecular Orbital (MO) theory – MO theory of H_2^+ ion, MO theory of H_2 molecule, MO treatment of homonuclear diatomic molecules – Li_2, Be_2, C_2, N_2, O_2 & F_2 and hetero nuclear diatomic molecules – LiH, CO, NO & HF, bond order</p> <p>3.4. Spectroscopic term symbols for diatomic molecules; Comparison of MO and VB theories</p>	
Unit 4: Chemical Bonding in Polyatomic Molecules	8 Hours

<p>4.1. Hybridization – quantum mechanical treatment of sp, sp² & sp³ hybridisation.</p> <p>4.2. Semi empirical MO treatment of planar conjugated molecules – Hückel Molecular Orbital (HMO) theory of ethylene, butadiene & allylic anion,</p> <p>4.3. Charge distributions and bond orders from the coefficients of HMO, calculation of free valence, HMO theory of aromatic hydrocarbons (benzene);</p> <p>4.4. Formula for the roots of the Hückel determinantal equation, Frost -Hückel circle mnemonic device for cyclic polyenes.</p>	
<p>Unit 5: Introduction to Computational Chemistry - I</p>	<p>8 Hours</p>
<p>5.1. Electronic structure of molecules – Basics of HF-SCF method of molecules (derivation not required).</p> <p>5.2. Classification of Computational Chemistry methods – Molecular mechanics methods (concept of force field) and electronic structure methods</p> <p>5.3. Ab initio and semi-empirical methods (Basic idea only), concept of electron correlation and post HF methods. (Elementary idea)</p>	
<p>Unit 6: Introduction to Computational Chemistry – II</p>	<p>8 Hours</p>
<p>6.1. Basis set approximation in ab initio methods -classification of basis sets – minimal, double zeta, triple zeta, split-valence, polarization & diffuse basis sets.</p> <p>6.2. Pople-style basis sets and their nomenclature.</p> <p>6.3. Simple calculations using Gaussian programme</p> <p>6.4. The structure of a Gaussian input file, Types of key words,</p> <p>6.5. Specification of molecular geometry using (a) Cartesian coordinates and (b) Internal coordinates.</p> <p>6.6. The Z-matrix - Z- matrices of some simple molecules like H₂, H₂O, formaldehyde, cis and trans H₂O₂, and NH₃.</p>	

MODE OF TRANSACTION

Face to Face Instruction: This involves attending traditional classroom lectures and participating in in-person discussions and activities with the instructor and fellow students.

Peer to Peer learning: Students have to select a topic in the course and present it in the class which providing opportunity for critical thinking and feedback.

Group Discussion: Group discussion will be conducted based on the relevant topic in the course that will improve students' thinking and help them to construct their own meaning about academic contents.

MODE OF ASSESSMENT					
Internal Assessment (15 Weightage)					
a. Internal Examination		2 Weightage			
<i>2 Internal Examinations, both should be considered</i>					
b. Assignments and Exercises:		3 Weightage			
c. Seminar/ Viva Voce:		3 Weightage			
d. Attendance:		3 Weightage			
External Assessment (30 Weightages) <i>Duration 3 Hours, No of Questions: 23</i>					
PATTERN OF QUESTION PAPER					
Division	Type	Total No. of questions	No. of questions to be answered	Weightages for each question	Total Weightage
Section A	Short	12	8	1	8
Section B	Short Essay	7	4	3	12
Section C	Essay	4	2	5	10
Total					30

MODULE WISE WEIGHTAGE DISTRIBUTION

Module	Mark
Unit 1: Thermodynamics	7
Unit 2: Thermodynamics of Irreversible Processes	8
Unit 3: Chemical Kinetics	8
Unit 4: Molecular Reaction Dynamics	8
Unit 5: Surface Chemistry	8
Unit 6: Catalysis	7

REFERENCES:

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M.Sc. CHEMISTRY (CBCSS PATTERN)
SEMESTER II

COURSE CODE –MCH2C06 COORDINATION CHEMISTRY				
Credit	Hours/week	Weightage		
		Internal	External	Total
3	3	5	30	35

Course Outcomes

CO No.	Expected Course Outcome	Learning Domain	PSO No
	Upon completion of this course, students will be able to;		
CO1	<i>Identify</i> ligand types	Remember	PSO 1
CO2	<i>Compare</i> strength of complexes	Evaluate	PSO 3
CO3	<i>Summarize</i> reactions of complexes	Understand	PSO 8
CO4	<i>Construct</i> diagrams of electronic transitions	Create	PSO 3
CO5	<i>Illustrate</i> Electron transfer mechanisms	Analyse	PSO 2
CO6	<i>Classify</i> types of photochemical reactions.	Understand	PSO 1
CO7	Distinguish structure from spectra	Analyse	PSO 3
CO8	<i>Judge</i> magnetic behaviour of lanthanoids and actinoids.	Evaluate	PSO 10
CO9	<i>Differentiate</i> photochemical reactions	Analyze	PSO 6
CO10	<i>Illustrate</i> redox properties in the excited states	Analyse	PSO 3

COURSE CONTENT

Unit 1: Stability of Co-ordination Compounds	5 Hours
<p>1.1. Stereochemistry of coordination compounds. Stepwise and overall formation constants and the relationship between them.</p> <p>1.2. Trends in stepwise formation constants.</p> <p>1.3. Determination of binary formation constants by pH-metry and spectrophotometry.</p> <p>1.4. Stabilisation of unusual oxidation states.</p> <p>1.5. Ambidentate and macrocyclic ligands.</p> <p>1.6. Chelate effect and its thermodynamic origin. Macrocyclic and template effects.</p>	
Unit 2: Theories of Bonding in Coordination Compounds	8 Hours
<p>2.1. Sidgwick's electronic interpretation of coordination. The valence bond theory and its limitations.</p> <p>2.2. The crystal field and ligand field theories. Splitting of d orbitals in octahedral, tetrahedral, square planar, square pyramidal and trigonal bipyramidal fields, LFSE, Dq values</p> <p>2.3. Jahn Teller (JT) effect</p> <p>2.4. Theoretical failure of crystal field theory, evidence of covalency in the metal-ligand bond, nephelauxetic effect</p> <p>2.5. Ligand field theory, molecular orbital theory- M.O energy level diagrams for octahedral and tetrahedral complexes without and with π-bonding, experimental evidences for pi-bonding.</p>	
Unit 3: Spectral and Magnetic Properties of Complexes	8 Hours
<p>3.1. Electronic Spectra of complexes: Term symbols of dn system, Racah parameters, splitting of terms in weak and strong octahedral and tetrahedral fields, d-d transitions, selection rules for electronic transitions-effect of spin orbit coupling and vibronic coupling.</p> <p>3.2. Interpretation of electronic spectra of complexes: Orgel diagrams and demerits, Tanabe-Sugano diagrams, calculation of Dq, B and β (Nephelauxetic</p>	

<p>ratio) values, spectra of complexes with lower symmetries, charge transfer spectra, luminescence spectra.</p> <p>3.3. Temperature independent paramagnetism (TIP), magnetic properties of lanthanoid and actinoid complexes spin state cross over.</p>	
Unit 4: Coordination Chemistry of Lanthanoids and Actinoids	5 Hours
<p>4.1. Term symbols for lanthanide ions, inorganic compounds and coordination complexes of the lanthanoids</p> <p>4.2. Electronic spectra and, general characteristics of actinoid- difference between 4f and 5f orbitals, coordination complexes of the actinoids</p> <p>4.3. Comparative account of coordination chemistry of lanthanoids and actinoids with special reference to electronic spectra and magnetic properties.</p>	
Unit 5: Characterization of Coordination Complexes	8 Hours
<p>5.1. Infrared spectra of metal complexes. Group frequency concept. Changes in ligand vibrations on coordination- metal ligand vibrations (Carbonyls, thiocyanates, nitro).</p> <p>5.2. Application in coordination complexes.</p> <p>5.3. ESR spectra – application to copper complexes.</p> <p>5.4. NMR spectroscopy for structural studies of diamagnetic metal complexes from chemical shift and spin- spin coupling.</p> <p>5.5. Mossbauer spectroscopy- Mossbauer Effect, hyperfine interactions (qualitative treatment).</p> <p>5.6. Application to iron and tin compounds.</p>	
Unit 6: Kinetics and Mechanism of Reactions in Metal Complexes	8 Hours
<p>6.1. Thermodynamic and kinetic stability, kinetics and mechanism of nucleophilic substitution reactions in square planar complexes</p> <p>6.2. Trans effect-theory and applications</p> <p>6.3. Kinetics and mechanism of octahedral substitution- water exchange, dissociative and associative mechanisms, base hydrolysis, racemization reactions, solvolytic reactions (acidic and basic).</p>	

<i>2 Internal Examinations, both should be considered</i>					
b. Assignments and Exercises:		3 Weightage			
c. Seminar/ Viva Voce:		3 Weightage			
d. Attendance:		3 Weightage			
External Assessment (30 Weightages) <i>Duration 3 Hours, No of Questions: 23</i>					
PATTERN OF QUESTION PAPER					
Division	Type	Total No. of questions	No. of questions to be answered	Weightages for each question	Total Weightage
Section A	Short	12	8	1	8
Section B	Short Essay	7	4	3	12
Section C	Essay	4	2	5	10
Total					30

MODULE WISE WEIGHTAGE DISTRIBUTION	
Module	Mark
Unit 1: Stability of Co-ordination Compounds	4
Unit 2: Theories of Bonding in Coordination Compounds	8
Unit 3: Spectral and Magnetic Properties of Complexes	8
Unit 4: Coordination Chemistry of Lanthanoids and Actinoids	5
Unit 5: Characterization of Coordination Complexes	8
Unit 6: Kinetics and Mechanism of Reactions in Metal Complexes	8
Unit 7: Redox and Photochemical Reactions of Complexes	5

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M.Sc. CHEMISTRY (CBCSS PATTERN)
SEMESTER II

COURSE CODE –MCH2C07 REACTION MECHANISM IN ORGANIC CHEMISTRY				
Credit	Hours/week	Weightage		
		Internal	External	Total
3	3	5	30	35

Course Outcomes

CO No.	Expected Course Outcome	Learning Domain	PSO No
	Upon completion of this course, students will be able to;		
CO1	<i>Classify</i> the different mechanisms of substitution reactions eliminations reactions.	Understand	PSO 2
CO2	<i>Compare</i> the mechanism and influence of conditions in each type reactions.	Evaluate	PSO 2
CO3	<i>Summarize</i> the mechanisms of different types of pericyclic and photochemical reactions organic chemistry	Understand	PSO 2
CO4	<i>Judge</i> the mechanism of pericyclic reactions through problem solving	Evaluate	PSO 5
CO5	<i>Interrelate</i> different types of mechanisms of carbonyl compounds	Understand	PSO 2
CO6	<i>Identify</i> the reactive intermediates in Molecular Rearrangements and Transformations	Remember	PSO 1
CO7	<i>Develop</i> suitable conditions for particular reactions by applying mechanistic aspects.	Create	PSO 7

COURSE CONTENT

Unit 1: Aliphatic and Aromatic Substitutions	8 Hours
<p>1.1. Nucleophilic Aliphatic Substitution: Mechanism and Stereochemistry of S_N2 and S_N1 reactions. Ion pair mechanism. The effect of substrate structure, reaction medium, nature of leaving group and nucleophile on S_N2 and S_N1 reactions.</p> <p>1.2. S_Ni and neighbouring group mechanism. SET mechanism. Allylic and benzylic substitutions. Ambident nucleophiles and substrates regioselectivity.</p> <p>1.3. Electrophilic Aliphatic Substitution: Mechanism and stereochemistry of SE_1, SE_2 (front), SE_2 (back) and SE_i reactions. The effect of substrate structure, leaving group and reaction medium on SE_1 and SE_2 reactions.</p> <p>1.4. Electrophilic Aromatic Substitution: Arenium ion mechanism, substituent effect on reactivity in mono and disubstituted benzene rings, <i>ortho/para</i> ratio, <i>Ipsso</i> substitution. Relationship between reactivity and selectivity.</p> <p>1.5. Nucleophilic Aromatic substitution: Addition-elimination (S_NAr) mechanism, elimination-addition (benzyne) mechanism, <i>cine</i> substitution, S_N1 and SRN_1 mechanism. The effect of substrate structure, nucleophile and leaving group on aromatic nucleophilic substitution.</p>	
Unit 2: Addition & Elimination Reactions and Reactive Intermediates	8 Hours
<p>2.1. Mechanistic and stereochemical aspects of addition to $C=C$ involving electrophiles, nucleophiles and free radicals. Effect of substituents on rate of addition, orientation of addition, addition to conjugated systems and cyclopropane rings, Michael reaction.</p> <p>2.2. Mechanistic and stereochemical aspects of E_1, E_1cB and E_2 eliminations. The effect of substrate structure, base, leaving group and reaction medium on elimination reactions. Saytzev elimination, Hofmann elimination, α-elimination, pyrolytic syn elimination (E_i) and conjugate eliminations. Competition between substitution and elimination reactions, basicity vs nucleophilicity. Extrusion reactions-extrusion of N_2, CO and CO_2.</p>	

2.3. Reactive Intermediates: Generation, geometry, stability and reactions of carbonium ions and carbanions, free radicals, carbenes, nitrenes and benzyenes.	
Unit 3: Chemistry of Carbonyl Compounds	8 Hours
<p>3.1. Reactions of Carbon-heteromultiple Bonds: Reactivity of carbonyl compounds toward addition, mechanistic aspects of hydration, addition of alcohols, and condensation with nitrogen nucleophiles to aldehydes and ketones.</p> <p>3.2. Addition of organometallic reagents- Grignard reagents- organozinc, organocopper and organolithium reagents- to carbonyl compounds. Aldol, Perkin, Claisen, Dieckmann, Stobbe and benzoin condensation. Darzen's, Knoevenagel, Reformatsky, Wittig, Cannizaro, Mannich and Prins reactions. MPV reduction and Oppenauer oxidation.</p> <p>3.3. Addition to carbon-nitrogen multiple bond: Ritter reaction and Thorpe condensation. Hydrolysis, alcoholysis and reduction of nitriles.</p> <p>3.4. Esterification and Ester Hydrolysis: Mechanisms of ester hydrolysis and esterification, Acyl-oxygen and alkyl oxygen cleavage.</p>	
Unit 4: Pericyclic Reactions	8 Hours
<p>4.1. Phase and symmetry of molecular orbitals, FMOs of ethylene, 1,3-butadiene, 1,3,5- hexatriene, allyl and 1,3-pentadienyl systems.</p> <p>4.2. Pericyclic reactions: electrocyclic, cycloaddition, sigmatropic, chelotropic and group transfer reactions.</p> <p>4.3. Theoretical models of pericyclic reactions: TS aromaticity method (Dewar-Zimmerman approach), FMO method and Correlation diagram method (Woodward-Hoffmann approach).</p> <p>4.4. Woodward- Hoffmann selection rules for electrocyclic, cycloaddition and sigmatropic reactions.</p> <p>4.5. Stereochemistry of Diels-Alder reactions and regioselectivity.</p> <p>4.6. Cope and Claisen rearrangements. Stereochemistry of cope rearrangement and valence tautomerism. 1,3- dipolar cycloaddition reactions and <i>ene</i> reactions.</p>	
Unit 5: Photochemistry of Organic Compounds	8 Hours

<p>5.1. Photochemical excitation of molecules, spin multiplicity, Jablonski diagram, photosensitization and quenching.</p> <p>5.2. Photochemistry of carbonyl compounds: Norrish type-I cleavage of acyclic, cyclic and β, γ-unsaturated carbonyl compounds, β- cleavage, γ- hydrogen abstraction: Norrish type-II cleavage, photo reduction, photoenolization.</p> <p>5.3. Photocyclo-addition of ketones with unsaturated compounds: Paterno-Büchi reaction, photodimerisation of α, β-unsaturated ketones,</p> <p>5.4. Photo rearrangements: Photo –Fries, di-π- methane, lumiketone, oxa di-π-methane rearrangements. Barton and Hoffmann-Loeffler-Freytag reactions.</p> <p>5.5. Photo isomerisation and dimerisation of alkenes, photo isomerisation of benzene and substituted benzenes, photooxygenation.</p>	
Unit 6: Molecular Rearrangements and Transformations	8 Hours
<p>6.1. Rearrangements occurring through carbocations, carbanions, carbenes and nitrenes such as Wagner-Meerwein, Demjanov, dienone-phenol, benzyl-benzilic acid, Favorskii, Wolff, Hofmann, Curtius, Lossen, Schmidt, Beckmann, Fries, Bayer-Villiger, Wittig, Orton, and Fries rearrangements.</p> <p>6.2. Peterson reaction, Woodward and Prevost hydroxylation reactions.</p> <p>6.3. Heck, Negishi, Sonogashira, Stille, and Suzuki coupling reactions (mechanism only).</p>	

MODE OF TRANSACTION
<p>Face to Face Instruction: This involves attending traditional classroom lectures and participating in in-person discussions and activities with the instructor and fellow students.</p> <p>Peer to Peer learning: Students have to select a topic in the course and present it in the class which providing opportunity for critical thinking and feedback.</p>

Unit 5: Photochemistry of Organic Compounds	9
Unit 6: Molecular Rearrangements and Transformations	9

REFERENCES:

1. M. B. Smith and J. March, *March's Advanced Organic Chemistry*, 6/e, John Wiley & Sons, 2007.
2. F. A. Carey and R. J. Sundburg, *Advanced Organic Chemistry, Part A & B*, 5/e, Springer, 2007.
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17. N. R. Krishnaswamy, Chemistry of Natural Products: A Laboratory Hand Book, 2/e, Universities Press.

M.Sc. CHEMISTRY (CBCSS PATTERN)
SEMESTER II

COURSE CODE –MCH2C08				
ELECTROCHEMISTRY, SOLID STATE CHEMISTRY AND STATISTICAL THERMODYNAMICS				
Credit	Hours/week	Weightage		
		Internal	External	Total
3	3	5	30	35

Course Outcomes

CO No.	Expected Course Outcome	Learning Domain	PSO No
	Upon completion of this course, students will be able to;		
CO1	<i>Identify</i> crystal systems.	Remember	PSO 1
CO2	<i>Compare</i> distribution functions	Evaluate	PSO 3
CO3	<i>Summarize</i> properties of solids	Understand	PSO 8
CO4	<i>Construct</i> stereographic projections	Create	PSO 3
CO5	<i>Illustrate</i> ionic interactions	Analyse	PSO 2
CO6	<i>Classify</i> point groups of solids	Understand	PSO 1
CO7	<i>Distinguish</i> reference electrodes	Analyse	PSO 3
CO8	<i>Judge</i> choice of fuel cells .	Evaluate	PSO 3
CO9	<i>Differentiate</i> magnetic properties of substances.	Analyse	PSO 6
CO10	<i>Outline</i> polarographic technique.	Analyse	PSO 5

COURSE CONTENT

Unit 1: Ionic Interaction & Equilibrium Electrochemistry	8 Hours
<p>1.1. The nature of electrolytes, Ion activity, Ion-ion and ion-solvent interaction, The electrical potential in the vicinity of an ion, Electrical potential and thermodynamic functions.</p> <p>1.2. The Debye-Hückel equation, Limiting and extended forms of the Debye-Hückel equation, Applications of the Debye-Hückel equation for the determination of thermodynamic equilibrium constants and to calculate the effect of ionic strength on ion reaction rates in solution</p> <p>1.3. Origin of electrode potentials-half cell potential-standard hydrogen electrode, reference electrodes- electrochemical series, applications- cell potential, Nernst equation for electrode and cell potentials, Nernst equation for potential of hydrogen electrode and oxygen electrode- thermodynamics of electrochemical cells, efficiency of electrochemical cells and comparison with heat engines</p> <p>1.4. Primary cells (Zn, MnO₂) and secondary cells (lead acid, Ni-Cd and Ni-MH cells), electrode reactions, potentials and cell voltages, advantages and limitations three types of secondary cells.</p> <p>1.5. Fuel cells; polymer electrolyte fuel cell (PEMFCs), alkaline fuel cells (AFCs), phosphoric acid fuel cells (PAFCs), direct methanol fuel cells, electrode reactions and potentials, cell reactions and cell voltages, advantages and limitations of four types of fuel cells</p>	
Unit 2: Dynamic Electrochemistry	8 Hours
<p>2.1. Electrical double layer-electrode kinetics of electrode processes, the Butler-Volmer equation-The relationship between current density and overvoltage, the Tafel equation. Polarization-electrolytic polarization, dissolution and deposition potentials, concentration polarization</p> <p>2.2. Overvoltage: hydrogen overvoltage and oxygen overvoltage: decomposition potential and overvoltage, individual electrode over voltages and its determination-metal deposition over voltage and its determination</p>	

<p>2.3. Theories of hydrogen overvoltage, the catalytic theory, the slow discharge theory, the electrochemical theory.</p> <p>2.4. Principles of polarography-dropping mercury electrode, the half wave potential.</p>	
<p>Unit 3: Solid State – I</p>	<p>8 Hours</p>
<p>3.1. Crystal symmetry: Symmetry elements and symmetry operations, mathematical proof for the non-existence of 5-fold axis of symmetry</p> <p>3.2. Crystal systems, Bravais lattices and crystal classes, Crystallographic point groups - Schönflies & Hermann–Mauguin notations,</p> <p>3.3. Stereographic projections of the 27 axial point groups</p> <p>3.4. Translational symmetry elements & symmetry operations - screw axes and glide planes, introduction to space groups.</p> <p>3.5. Bragg’s law and applications, lattice planes and miller indices, d-spacing formulae, crystal densities and unit cell contents</p> <p>3.6. Imperfections in solids - point, line and plane defects, non-stoichiometry.</p>	
<p>Unit 4: Solid State – II</p>	<p>8 Hours</p>
<p>4.1. Electronic structure of solids – free electron theory, band theory & Zone theory, Brillouin zones;</p> <p>4.2. Electrical properties - electrical conductivity, Hall effect, dielectric properties, piezo electricity, ferro-electricity, and ionic conductivity</p> <p>4.3. Superconductivity- Meissner effect, brief discussion of Cooper theory of superconductivity.</p> <p>4.4. Optical properties - photo conductivity, luminescence, colour centres, lasers, refraction & birefringence.</p> <p>4.5. Magnetic properties - diamagnetism, paramagnetism, ferromagnetism, antiferromagnetism & ferrimagnetism</p> <p>4.6. Thermal properties - thermal conductivity and specific heat</p>	
<p>Unit 5: Statistical Thermodynamics- I</p>	<p>8 Hours</p>
<p>5.1. Fundamentals – concept of distribution, thermodynamic probability and most probable distribution, ensembles</p>	

<p>5.2. Statistical mechanics for systems of independent particles and its importance in chemistry, thermodynamic probability & entropy, idea of microstates and macrostates, statistical weight factor (g), Sterling approximation</p> <p>5.3. Maxwell- Boltzman statistics. The molecular partition function and its relation to the thermodynamic properties, derivation of third law of thermodynamics.</p> <p>5.4. Equilibrium- constant & equi-partition principle in terms of partition functions, relation between molecular & molar partition functions, factorisation of the molecular partition function into translational, rotational, vibrational and electronic parts, the corresponding contributions to the thermodynamic properties</p> <p>5.5. Evaluation of partition functions and thermodynamic properties for ideal mono-atomic and diatomic gases.</p>	
<p>Unit 6: Statistical Thermodynamics- II</p>	<p>8 Hours</p>
<p>6.1. Heat capacities of solids - classical and quantum theories, Einstein's theory of atomic crystals and Debye's modification.</p> <p>6.2. Quantum Statistics: Bose - Einstein distribution law, Bose-Einstein condensation, application to liquid helium; Fermi - Dirac distribution law, application to electrons in metals</p> <p>6.3. Relationship between Maxwell-Boltzman, Bose-Einstein, and Fermi-Dirac statistics.</p>	

<p>MODE OF TRANSACTION</p>
<p>Face to Face Instruction: This involves attending traditional classroom lectures and participating in in-person discussions and activities with the instructor and fellow students.</p> <p>Peer to Peer learning: Students have to select a topic in the course and present it in the class which providing opportunity for critical thinking and feedback.</p>

Unit 5: Statistical Thermodynamics- I	9
Unit 6: Statistical Thermodynamics- II	9

REFERENCES:

1. N.N. Greenwood and A. Earnshaw, Chemistry of Elements, 2/e, Elsevier Butterworth- Heinemann, 2005.
2. J.E. Huheey, E.A. Keiter, R.L. Keiter. O.K. Medhi. Inorganic Chemistry, Principles of structure and reactivity, Pearson Education, 2006.
3. G.L. Miessler, D.A. Tarr, Inorganic Chemistry, Pearson, 2010.
4. D.F. Shriver, P.W. Atkins, Inorganic Chemistry, Oxford University Press, 2002
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6. Keith F Purcell, John C Kotz, Inorganic Chemistry, Cengage Learning, 2010.
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9. R.L. Dutta and A. Shyamal, Elements of Magnetochemistry, SChand and Co. 1982.
10. H.J. Arnikar, Essentials of Nuclear chemistry, New Age International, 2005.
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M.Sc. CHEMISTRY (CBCSS PATTERN)
SEMESTER I & II

COURSE CODE –MCH1L01 & MCH2L04				
INORGANIC CHEMISTRY PRACTICALS– I & II				
Credit	Hours/week	Weightage		
		Internal	External	Total
3	4	10	30	40

Course Outcomes

CO No.	Expected Course Outcome	Learning Domain	PSO No.
	Upon completion of this course, students will be able to;		
CO1	<i>Recall</i> and <i>explain</i> the principles involved in inorganic qualitative and qualitative analysis	Remember	PSO6
CO2	<i>Apply</i> the concepts like common ion effect and solubility product principle in analyzing cations	Apply	PSO4
CO3	<i>Analyze</i> common and less familiar cations	Analyze	PSO4
CO4	<i>Develop</i> laboratory competence in relating chemical structures using spectroscopy	Create	PSO9
CO5	<i>Measure</i> the quantity of different ions using colorimetry	Evaluate	PSO5
CO6	<i>Develop</i> critical thinking and analysis skill to solve complex inorganic problems	Analyze	PSO3 PSO5 PSO6

COURSE CONTENT

Experiment	128 Hours
Unit 1: Inorganic Cation Mixture Analysis	
<p>1.1. Separation and identification of four metal ions of which two are less-familiar elements like W, Se, Te, Mo, Ce, Th, Ti, Zr, V, U and Li. (Eliminating acid radicals not present).</p> <p>1.2. Confirmation by spot tests and comparison with heat engines</p>	
Unit 2: Volumetric Analysis	
<p>2.1. Volumetric Determinations using: EDTA (Al, Ba, Ca, Cu, Fe, Ni, Co, hardness of water)</p> <p>2.2. Cerimetry (Fe^{2+}, nitrite)</p> <p>2.3. Potassium Iodate (Iodide, Sn^{2+})</p>	
Unit 3: Colorimetric Analysis	
3.1. Colorimetric Determinations of metal ions Fe, Cr, Ni, Mn and	

Mode of Transaction
<p>Demonstrations: Helps to illustrate and consolidate theoretical principles outlined in the course.</p> <p>Experimentation: This involves learning by doing or hands on experience by applying chemical principles.</p> <p>Observation: It involves noticing or perceiving the course of the experiment or measurement by equipment and acquisition of information from the primary source:</p>

Mode of Assessment
Internal Assessment (10 Weightage)

a. Attendance:	2 weightage
b. Lab skill/quality of their results:	2 weightage
c. Model practical test:	2 weightage
<i>(Best one, out of two model exams is considered)</i>	
d. Record:	2 weightage
e. Viva Voce:	2 weightage
External Assessment (30 Weightage)	

SEE will be at the end of the second semester.

REFERENCES:

1. G.H. Jeffery, J. Basseett, J. Mendham and R.C. Denny, Vogel's Textbook of Quantitative Chemical Analysis, 5th Edition, ELBS, 1989.
2. D.A. Skoog and D.M. West, Analytical Chemistry, An Introduction, 4th Edition, CBS Publishing Japan Ltd., 1986.
3. E.J. Meehan, S. Bruckenstein and I.M. Kolthoff and E.B. Sandell, Quantitative Chemical Analysis, 4th Edition, The Macmillan Company, 1969.
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M.Sc. CHEMISTRY (CBCSS PATTERN)
SEMESTER I & II

COURSE CODE –MCH1L02 & MCH2L05 ORGANIC CHEMISTRY PRACTICALS– I & II				
Credit	Hours/week	Weightage		
		Internal	External	Total
3	4	10	30	40

Course Outcomes

CO No.	Expected Course Outcome	Learning Domain	PSO No.
	Upon completion of this course, students will be able to;		
CO1	<i>Recall</i> and explain the principles involved in organic qualitative and qualitative analysis	Remember	PSO6
CO2	<i>Apply</i> the concepts like solvent polarity in the separation of organic mixtures	Apply	PSO4
CO3	<i>Analyse</i> and identify organic compounds with more than one functional group.	Analyse	PSO4
CO4	<i>Develop</i> laboratory competence in relating chemical structures using spectroscopy	Create	PSO9
CO5	<i>Prepare</i> and measure the yield of organic compounds.	Evaluate	PSO5
CO6	<i>Develop</i> and create methods to synthesis novel organic compounds.	Create	PSO3 PSO5 PSO6

COURSE CONTENT

Experiment	128 Hours
Unit 1: Laboratory Techniques	
1.1. Methods of Separation and Purification of Organic Compounds – fractional, steam and low-pressure distillations, fractional crystallisation and sublimation	
Unit 2: Separation and identification of the components of organic binary mixtures	
2.1. Microscale analysis is preferred. Analysis of about ten binary mixtures, some of which containing compounds with more than one functional group.	
2.2. Separation and identification of a few ternary mixtures.	
Unit 3: Organic preparations	
3.1. Double stage (minimum six)	
3.2. Three stage (minimum two)	

Mode of Transaction

Demonstrations: Helps to illustrate and consolidate theoretical principles outlined in the course.

Experimentation: This involves learning by doing or hands on experience by applying chemical principles.

Observation: It involves noticing or perceiving the course of the experiment or measurement by equipment and acquisition of information from the primary source:

Mode of Assessment

Internal Assessment (10 Weightage)

- a. Attendance: 2 weightage

b. Lab skill/quality of their results:	2 weightage
c. Model practical test:	2 weightage
<i>(Best one, out of two model exams is considered)</i>	
d. Record:	2 weightage
e. Viva Voce:	2 weightage
External Assessment (30 Weightage)	

SEE will be at the end of the second semester.

REFERENCES:

1. B.S. Furnis, A.J. Hannaford, P.W.G. Smith and A.R. Tatchell, Vogel's Textbook of Practical Organic Chemistry, 5/e, Pearson, 1989.
2. Shriner, Fuson and Curtin, Systematic Identification of Organic Compounds, 1964. Fieser, Experiments in Organic Chemistry, 1957.
3. Dey, Sitaraman and Govindachari, A Laboratory Manual of Organic Chemistry, 3rd Edition, 1957.
4. P.R. Singh, D.C. Gupta and K.S. Bajpal, Experimental Organic Chemistry, Vol. I and II, 1980.
5. Vishnoi, Practical Organic Chemistry. Pavia, Kriz, Lampman, and Engel, A Microscale Approach to Organic Laboratory Techniques, 5/e, Cengage, 2013.
6. Mohrig, Hammond and Schatz, Techniques in Organic Chemistry: Miniscale, Standard Taper Microscale and Williamson Microscale, 3/e, W. H. Freeman and Co., 2010.

M.Sc. CHEMISTRY (CBCSS PATTERN)
SEMESTER I & II

COURSE CODE –MCH1L03 & MCH2L06				
PHYSICAL CHEMISTRY – I & II				
Credit	Hours/week	Weightage		
		Internal	External	Total
3	4	10	30	40

Course Outcomes

CO No.	Expected Course Outcome	Learning Domain	PSO No.
	Upon completion of this course, students will be able to;		
CO1	<i>Develop</i> analytical skills in determining the physical properties (physical constants).	Create	PSO4
CO2	<i>Develop</i> skill in setting up an experimental method to determine the physical properties.	Create	PSO4
CO3	<i>Estimate</i> physical parameters	Understand	PSO6
CO4	<i>Explain</i> the principles of Viscometry, Refractometry, Potentiometry and Conductometry; and to apply the skill to determine unknown concentration	Understand Apply	PSO6
CO5	<i>Demonstrate</i> the principles of Solubility, Phase equilibria and Distribution Law	Understand	PSO5
CO6	<i>Interpret</i> the measured data and draw conclusion	Understand Evaluate	PSO5
CO7	<i>Calculate</i> various physical parameters	Apply	PSO5

COURSE CONTENT

Experiment	128 Hours
Unit 1: Solubility and Heat of solution (<i>minimum 2 experiments</i>)	
1.1. Determination of molar heat of solution of a substance (e.g., ammonium oxalate, succinic acid) from solubility data - analytical method and graphical method	
Unit 2: Phase Equilibria (<i>minimum 3 experiments</i>)	
2.1. Determination of phase diagram of a simple eutectic system (e.g., Biphenyl, Naphthalene- Diphenyl amine)	
2.2. Determination of the composition of a binary solid mixture.	
2.3. Determination of phase diagram of a binary solid system forming a compound (e.g., Naphthalene – m-dinitrobenzene).	
Unit 3: Viscosity (<i>minimum 2 experiments</i>)	
3.1. Viscosity of mixtures - Verification of Kendall's equation (e.g., benzene - nitrobenzene, water-alcohol).	
3.2. Determination of molecular weight of a polymer (e.g., polystyrene in	
Unit 4: Distribution Law (<i>minimum 3 experiments</i>)	
4.1. Determination of distribution coefficient of I ₂ between CCl ₄ and H ₂ O.	
4.2. Determination of equilibrium constant of KI + I ₂ = KI ₃	
4.3. Determination of concentration of KI solution	
Unit 5: Refractometry (<i>minimum 3 experiments</i>)	
5.1. Determination of molar refractions of pure liquids (e.g., water, methanol, ethanol, chloroform, carbon tetrachloride, glycerol)	
5.2. Determination of composition of liquid mixtures (e.g., alcohol -water, glycerol-water)	
5.3. Determination of molar refraction and refractive index of a solid	

Unit 6: Conductivity (*minimum 4 experiments*)

- 6.1. Determination of equivalent conductance of a weak electrolyte (e.g.,
- 6.2. acetic acid), verification of Ostwald's dilution law and calculation of dissociation constant.
- 6.3. Determination of solubility product of a sparingly soluble salt (e.g., AgCl, BaSO₄)
- 6.4. Conductometric titrations- HCl vs NaOH, (HCl + CH₃-COOH) vs NaOH
- 6.5. Determination of the degree of hydrolysis of aniline hydrochloride

Unit 7: Potentiometry (*minimum 3 experiments*)

- 7.1. Potentiometric titration: HCl vs NaOH, CH₃-COOH vs NaOH
- 7.2. Redox titration: KI vs KMnO₄, FeSO₄ vs K₂Cr₂O₇
- 7.3. Determination of dissociation constant of acetic acid by potentiometric titration
- 7.4. Determination of pH of weak acid using Potentiometry
- 7.5. Determination of pH of acids and bases using pH meter

Mode of Transaction

Demonstrations: Helps to illustrate and consolidate theoretical principles outlined in the course.

Experimentation: This involves learning by doing or hands on experience by applying chemical principles.

Observation: It involves noticing or perceiving the course of the experiment or measurement by equipment and acquisition of information from the primary source:

Mode of Assessment

Internal Assessment (10 Weightage)

- a. Attendance: 2 weightage

b. Lab skill/quality of their results:	2 weightage
c. Model practical test:	2 weightage
<i>(Best one, out of two model exams is considered)</i>	
d. Record:	2 weightage
e. Viva Voce:	2 weightage
External Assessment (30 Weightage)	

SEE will be at the end of the second semester.

References:

1. J.B. Firth, Practical Physical Chemistry, Read Books (Reprint 2008).
2. A Finlay, Practical Physical Chemistry, Longman's Green & Co.
3. A.M. James, Practical Physical Chemistry, Longman, 1974.
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7. D.P. Shoemaker and C.W. Garland, Experimental Physical Chemistry, McGraw Hill.
8. J. B. Yadav, Advanced Practical Physical Chemistry, Goel Publications, 1989.
9. B. Viswanathan & R.S. Raghavan, Practical Physical Chemistry, Viva Books, 2009.
10. G. Brauer, Handbook of Preparative Inorganic Chemistry.

M.Sc. CHEMISTRY (CBCSS PATTERN)
SEMESTER III

COURSE CODE –MCH3C09 MOLECULAR SPECTROSCOPY				
Credit	Hours/week	Weightage		
		Internal	External	Total
4	4	5	30	35

Course Outcomes

CO No.	Expected Course Outcome	Learning Domain	PSO No
	Upon completion of this course, students will be able to		
CO1	Understand the quantum chemical principles through spectroscopy	Understand	PSO 1 PSO 8
CO2	<i>Identify</i> basic physical chemistry law that govern molecular spectroscopy	Remember	PSO 3
CO3	<i>Summarize</i> the basic information on molecular spectroscopic methods (IR, Raman, UV-VIS, NMR, EPR)	Understand	PSO 8
CO4	<i>Select</i> the molecular spectroscopy methods for solving given scientific problem	Create	PSO 3
CO5	<i>Analyse</i> various spectra of organic molecules and identify the differences	Analyse	PSO 2 PSO 3
CO6	<i>Distinguish</i> the importance of spectroscopic technique in material sciences	Analyse	PSO 3
CO7	Structural <i>determination</i> of organic compounds using spectroscopic techniques	Apply	PSO 8
CO8	<i>Evaluate</i> choice of suitable spectroscopic method for a organic molecule.	Evaluate	PSO 3, PSO 10

COURSE CONTENT

Unit 1: Basic Aspects and Microwave Spectroscopy - Theory only	8 Hours
<p>1.1. Electromagnetic radiation & its different regions, Interaction of matter with radiation and its effect on the energy of a molecule, Factors affecting the width and Intensity of Spectral lines.</p> <p>1.2. Microwave spectroscopy - Rotation spectra of diatomic and poly atomic molecules - rigid and non-rigid rotator models, asymmetric, symmetric and spherical tops, isotope effect on rotation spectra.</p> <p>1.3. Stark effect, nuclear and electron spin interactions, rotational transitions and selection rules, determination of bond length using microwave spectral data.</p>	
Unit 2: Infrared, Raman and Electronic Spectroscopy - Theory only	8 Hours
<p>2.1. Vibrational spectroscopy -Normal modes of vibration of a molecule; Vibrational spectra of diatomic molecules, anharmonicity, Morse potential, fundamentals, overtones, hot bands, combination bands, difference bands; Vibrational spectra of polyatomic molecules; Vibration- rotation spectra of diatomic and polyatomic molecules, spectral branches -P, Q & R branches.</p> <p>2.2. Attenuated total reflectance-Fourier transform infrared (ATR-FTIR) spectroscopy</p> <p>2.3. Raman spectroscopy –Classical and Quantum theory of Raman effect Pure rotational & pure vibrational Raman spectra, vibrational-rotational Raman spectra, selection rules, mutual exclusion principle; Introduction to Resonance Raman spectroscopy (basics only).</p> <p>2.4. Electronic Spectroscopy- Characteristics of electronic transitions – Vibrational coarse structure, intensity of electronic transitions, Franck - Condon principle, types of electronic transitions; Dissociation and predissociation; Ground and excited electronic states of diatomic molecules; Electronic spectra of polyatomic molecules; Electronic spectra of conjugated molecules.</p> <p>2.5. Fluorimetry: General discussion-relationship between intensity and concentration- applications</p>	

Unit 3: Magnetic Resonance Spectroscopy - Theory only	8 Hours
<p>3.1. NMR: Quantum mechanical description of Energy Levels -Population of energy-nuclear shielding- Chemical shift- Spin-Spin coupling and splitting of NMR signals- Quantum mechanical Description- AX and AB NMR pattern- Karplus relationship</p> <p>3.2. Nuclear Overhauser Effect- FT NMR- 2D NMR COSY</p> <p>3.3. Electron Spin Resonance: Quantum mechanical description of electron spin in a magnetic field- Energy levels-Population- Mc Connell Relation</p> <p>3.4. Equivalent and non-equivalent nucleus - g anisotropy.</p>	
Unit 4: NQR, Mossbauer and Surface Enhanced Raman Scattering	8 Hours
<p>4.1. Nuclear Quadrupole Resonance Spectroscopy: Principle, transitions for axially symmetric systems, transitions for Nonaxial symmetric systems, NQR group frequencies</p> <p>4.2. Mossbauer Spectroscopy: The Mossbauer effect, hyperfine interactions, isomer shift, electric quadrupole and magnetic hyperfine interactions.</p> <p>4.3. Surface Enhanced Raman Scattering: Introduction, Surfaces for SERS study, Surface Selection Rules, Representative Spectra, Applications of SERS</p>	
Unit 5: Electronic & Vibrational Spectroscopy in Organic Chemistry	8 Hours
<p>5.1. UV-Visible spectroscopy: Factors affecting the position and intensity of electronic absorption bands – conjugation, solvent polarity and steric parameters</p> <p>5.2. Empirical rules for calculating λ_{\max} of dienes, enones and benzene derivatives.</p> <p>5.3. Optical Rotatory Dispersion and Circular Dichroism: Linearly and circularly polarized lights, circular birefringence, ellipticity and circular dichroism, ORD and Cotton effect.</p> <p>5.4. Octant rule and Axial haloketone rule for the determination of conformation and Configuration of 3-methyl cyclohexanone and cis- and trans decalones. CD curves</p> <p>5.5. Infrared Spectroscopy: Functional group and fingerprint regions</p>	

<p>5.6. Factors affecting vibrational frequency: Conjugation, coupling, electronic, steric, ring strain and hydrogen bonding.</p> <p>5.7. Important absorption frequencies of different class of organic compounds- hydrocarbons, alcohols, thiols, carbonyl compounds, amines, nitriles</p>	
Unit 6: NMR Spectroscopy in Organic Chemistry - I	8 Hours
<p>6.1. ¹H NMR: Chemical shift, factors influencing chemical shift, anisotropic effect. Chemical shift values of protons in common organic compounds, Chemical, magnetic and stereochemical equivalence.</p> <p>6.2. Enantiotopic, diastereotopic and homotopic protons. Protons on oxygen and nitrogen. Quadrupole broadening. Spin – spin coupling, types of coupling.</p> <p>6.3. Coupling constant, factors influencing coupling constant, effects of chemical exchange, fluxional molecules, hindered rotation on NMR spectrum,</p> <p>6.4. First order and non-first order NMR spectra, Karplus relationship.</p>	
Unit 7: NMR Spectroscopy in Organic Chemistry - II	8 Hours
<p>7.1. Simplification of NMR spectra: double resonance, shift reagents, increased field strength, deuterium labelling. NOE spectra, heteronuclear coupling. Introduction to COSY, HMBC, HMQC spectra</p> <p>7.2. ¹³C NMR: General considerations, comparison with PMR, factors influencing carbon chemical shifts, carbon chemical shifts and structure-saturated aliphatics, unsaturated aliphatics, carbonyls, and aromatics.</p> <p>7.3. Off-resonance and noise decoupled spectra, Introduction to DEPT, INEPT, INADEQUATE.</p>	
Unit 8: Mass Spectrometry and Spectroscopy for Structure Elucidation	8 Hours
<p>8.1. Mass Spectrometry: Basic concept of EIMS. Molecular ion and meta stable ion peaks, Isotopic peaks. Molecular weight and molecular formula</p> <p>8.2. Single and multiple bond cleavage, rearrangements-McLafferty rearrangements.</p>	

- 8.3. Fragmentation pattern of some common organic compounds – saturated and unsaturated hydrocarbons, ethers, alcohols, aldehydes and ketones, amines and amides.
- 8.4. High resolution mass spectrometry, index of hydrogen deficiency, Nitrogen rule and Rule of Thirteen. Ionization techniques. FAB spectra.
- 8.5. Structural determination of organic compounds using spectroscopic techniques (Problem solving approach)

MODE OF TRANSACTION

Face to Face Instruction: This involves attending traditional classroom lectures and participating in in-person discussions and activities with the instructor and fellow students.

Peer to Peer learning: Students have to select a topic in the course and present it in the class which providing opportunity for critical thinking and feedback.

Group Discussion: Group discussion will be conducted based on the relevant topic in the course that will improve students' thinking and help them to construct their own meaning about academic contents.

MODE OF ASSESSMENT

Internal Assessment (15 Weightage)

- | | |
|---|-------------|
| a. Internal Examination | 2 Weightage |
| <i>2 Internal Examinations, both should be considered</i> | |
| b. Assignments and Exercises: | 3 Weightage |
| c. Seminar/ Viva Voce: | 3 Weightage |
| d. Attendance: | 3 Weightage |

External Assessment (30 Weightages) *Duration 3 Hours, No of Questions: 23*

PATTERN OF QUESTION PAPER

Division	Type	Total No. of questions	No. of questions to be answered	Weightages for each question	Total Weightage
Section A	Short	12	8	1	8
Section B	Short Essay	7	4	3	12
Section C	Essay	4	2	5	10
Total					30

MODULE WISE WEIGHTAGE DISTRIBUTION	
Module	Mark
Unit 1: Basic Aspects and Microwave Spectroscopy - Theory only	6
Unit 2: Infrared, Raman and Electronic Spectroscopy - Theory only	6
Unit 3: Magnetic Resonance Spectroscopy - Theory only	6
Unit 4: NQR, Mossbauer and Surface Enhanced Raman Scattering	7
Unit 5: Electronic & Vibrational Spectroscopy in Organic	7
Unit 6: NMR Spectroscopy in Organic Chemistry - I	7
Unit 7: NMR Spectroscopy in Organic Chemistry - II	7
Unit 8: Mass Spectrometry and Spectroscopy for Structure	7

REFERENCES:

1. G.M. Barrow, Introduction to Molecular Spectroscopy, McGraw Hill, 1962.
2. C.N. Banwell & E. M. McCash, Fundamentals of Molecular Spectroscopy, Tata McGraw Hill, New Delhi, 1994.
3. Thomas Engel, Quantum Chemistry & Spectroscopy, Pearson education, 2006.
4. P. Atkins & J. De Paula, Atkins's Physical Chemistry, 8th Edition, W.H. Freeman & Co., 2006.
5. D.A. McQuarrie and J.D. Simon, Physical Chemistry - A Molecular Approach, University Science Books, 1997.
6. D.N. Sathyanarayana, Electronic Absorption Spectroscopy and Related Techniques, University Press, 2000.
7. R.S. Drago, Physical methods for Chemists, Second edition, Saunders College

8. Publishing 1977 (For NMR and EPR, Mossbauer)
9. Gunther, NMR Spectroscopy: Basic Principles, Concepts and Applications in
10. Chemistry, 2/e, John Wiley
11. Ferraro, Nakamoto and Brown, Introductory Raman Spectroscopy, 2/e,
Academic Press, 2005.
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13. Silverstein, Spectrometric Identification of Organic Compounds, 6/e, John Wiley
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15. Jag Mohan, Organic Spectroscopy: Principles and Applications, 2/e, Narosa
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M.Sc. CHEMISTRY (CBCSS PATTERN)
SEMESTER III

COURSE CODE –MCH3C10				
ORGANOMETALLIC AND BIOINORGANIC CHEMISTRY				
Credit	Hours/week	Weightage		
		Internal	External	Total
4	3	5	30	35

Course Outcomes

CO No.	Expected Course Outcome	Learning Domain	PSO No.
	Upon completion of this course, students will be able to;		
CO1	<i>Identify</i> denticity and hapticity of ligands.	Remember	PSO 1
CO2	<i>Compare</i> storage and transport proteins	Evaluate	PSO 3
CO3	<i>Summarize</i> role of enzymes and coenzymes	Understand	PSO 8
CO4	<i>Illustrate</i> action of anti-cancer drugs	Analyse	PSO 2
CO5	<i>Classify</i> role of metal ions in biological systems	Understand	PSO 1
CO6	<i>Discriminate</i> role of the two photosystems	Analyse	PSO 3
CO7	<i>Judge</i> structure of clusters.	Evaluate	PSO 10
CO8	<i>Differentiate</i> magnetic properties of substances.	Analyse	PSO 6
CO9	<i>Categorize</i> reactions of organometallic compounds.	Analyse	PSO 6 PSO 5
CO10	<i>Indicate</i> fluxional isomerism	Understand	PSO 1
CO1	<i>Contrast</i> polymerization by different catalysts	Evaluate	PSO 11

COURSE CONTENT

Unit 1: Organometallic Compounds-Synthesis, Structure and Bonding	8 Hours
<p>1.1. Denticity and hapticity of common ligands, organometallic compounds with linear pi donor ligands-olefins, acetylenes, dienes and allyl complexes-</p> <p>1.2. Synthesis, structure and bonding. Synthesis and structure of complexes with cyclic pi donors, metallocenes and cyclic arene complexes</p> <p>1.3. Bonding in ferrocene and dibenzenechromium, carbene and carbyne complexes.</p>	
Unit 2: Metal clusters	8 Hours
<p>2.1. Metal carbonyls: CO as a π-bonding ligand, synergism, preparation, properties, structure and bonding of simple mono and binuclear metal carbonyls, metal nitrosyls, metal cyanides and dinitrogen complexes.</p> <p>2.2. Polynuclear metal carbonyls with and without bridging. Carbonyl clusters-LNCC and HNCC, Isoelectronic and isolobal analogy, Wade-Mingos rules, cluster valence electrons.</p> <p>2.3. IR spectral studies of bridging and non-bridging CO ligands. Carbide clusters.</p>	
Unit 3: Reactions of organometallic compounds and catalysis	10 Hours
<p>3.1. Organometallic reactions - ligand dissociation and substitution- Oxidative addition and reductive elimination. Insertion reactions involving CO and alkenes, α, β, γ and δ eliminations.</p> <p>3.2. Carbonylation by Collman's reagent. Electrophilic and Nucleophilic attack on coordinated ligand. Redistribution reactions</p> <p>3.3. Fluxional isomerism of allyl, cyclopentadienyl and allene systems.</p> <p>3.4. Homogeneous and heterogeneous catalysis: Tolman catalytic loops, alkene hydrogenation using Wilkinson catalyst, Hydroformylation of olefins using cobalt and rhodium catalysts, Wacker process, Monsanto acetic acid process, Cativa process and olefin metathesis.</p>	

<p>3.5. Heterogeneous catalysis by organometallic compounds: Polymerization by organometallic initiators and templates for chain propagation- Ziegler Natta catalysts, polymerisation by metallocene catalysts.</p> <p>3.6. Reactions of carbon monoxide and hydrogen-the water gas shift reaction, the Fischer- Tropsch reaction (synthesis of gasoline).</p>	
Unit 4: Organometallic Polymers	(6 hrs)
<p>4.1. Polymers with organometallic moieties as pendant groups,</p> <p>4.2. polymers with organometallic moieties in the main chain,</p> <p>4.3. condensation polymers based on ferrocene and on rigid rod polyynes,</p> <p>4.4. polymers prepared by ring opening polymerization, organometallic dendrimers.</p>	
Unit 5: Bioinorganic Chemistry-I	8 Hours
<p>5.1. Occurrence of inorganic elements in biological systems- bulk and trace metal ions. Emergence of bioinorganic chemistry. Coordination sites in biologically important ligands.</p> <p>5.2. Role of alkali metal ions in biological systems. Structural role of calcium.</p> <p>5.3. Storage and transport of metal ions- ferritin, transferrin and siderophores.</p> <p>5.4. Oxygen transport by heme proteins-hemoglobin and myoglobin-structure of the oxygen binding site-nature of heme-dioxygen binding-cooperativity. Hemerythrin and hemocyanin.</p> <p>5.5. Ion transport across membranes. The sodium/potassium pump.</p>	
Unit 6: Bioinorganic Chemistry-II	8 Hours
<p>6.1. Electron carrier proteins. Iron-Sulphur proteins and cytochromes. Metallo enzymes-Iron enzymes: Cytochrome P-450, catalase and peroxidase.</p> <p>6.2. Copper enzymes: Oxidase, superoxide dismutase and tyrosinase.</p> <p>6.3. Zinc enzymes: Carboxypeptidase and carbonic anhydrase.</p> <p>6.4. Cobalt enzymes Vitamin B12 and coenzymes. Vitamin B12 and coenzymes.</p> <p>6.5. Chlorophyll II- Photosystem I and II. Nitrogen fixation-Nitrogenases.</p> <p>6.6. Anticancer drugs. Action of Cis-platin.</p>	

MODE OF TRANSACTION

Face to Face Instruction: This involves attending traditional classroom lectures and participating in in-person discussions and activities with the instructor and fellow students.

Peer to Peer learning: Students have to select a topic in the course and present it in the class which providing opportunity for critical thinking and feedback.

Group Discussion: Group discussion will be conducted based on the relevant topic in the course that will improve students' thinking and help them to construct their own meaning about academic contents.

MODE OF ASSESSMENT

Internal Assessment (15 Weightage)

- | | |
|---|-------------|
| a. Internal Examination | 2 Weightage |
| <i>2 Internal Examinations, both should be considered</i> | |
| b. Assignments and Exercises: | 3 Weightage |
| c. Seminar/ Viva Voce: | 3 Weightage |
| d. Attendance: | 3 Weightage |

External Assessment (30 Weightages) *Duration 3 Hours, No of Questions: 23*

PATTERN OF QUESTION PAPER

Division	Type	Total No. of questions	No. of questions to be answered	Weightages for each question	Total Weightage
Section A	Short	12	8	1	8
Section B	Short Essay	7	4	3	12
Section C	Essay	4	2	5	10
Total					30

MODULE WISE WEIGHTAGE DISTRIBUTION	
Module	Mark
Unit 1: Organometallic Compounds-Synthesis, Structure and	8
Unit 2: Metal clusters	9
Unit 3: Reactions of organometallic compounds and catalysis	12
Unit 4: Organometallic Polymers	6
Unit 5: Bioinorganic Chemistry-I	9
Unit 6: Bioinorganic Chemistry-II	9

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3. G.L. Miessler, D.A. Tarr, Inorganic Chemistry, Pearson, 2010.
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11. P. Powell, Principles of Organometallic Chemistry, ELBS.
12. B.D. Gupta and A.J. Elias, Basic Organometallic Chemistry, Concepts, Synthesis and Applications, Universities Press, 2010.
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M.Sc. CHEMISTRY (CBCSS PATTERN)
SEMESTER III

COURSE CODE –MCH3C11				
REAGENTS AND TRANSFORMATIONS IN ORGANIC CHEMISTRY				
Credit	Hours/week	Weightage		
		Internal	External	Total
4	3	5	30	35

Course Outcomes

CO No.	Expected Course Outcome	Learning Domain	PSO No
	Upon completion of this course, students will be able to;		
CO1	<i>Identify</i> various reagents for specific organic conversions.	Remember	PSO 1
CO2	<i>Compare</i> the suitable reagents for various organic transformation	Evaluate	PSO 3
CO3	<i>Summarize</i> the organic transformations	Understand	PSO 2
CO4	<i>Explain</i> the mechanism and stereochemistry behind various reactions.	Create	PSO 7
CO5	<i>Illustrate</i> applications of various reagents	Analyse	PSO 2 PSO 3
CO6	<i>Classify</i> types of organic reactions	Understand	PSO 1
CO7	<i>Choose</i> the correct reagents for the specific transformations	Create	PSO 3 PSO7
CO8	<i>Summarize</i> the use of organometallic reagents carbon -carbon bond formations reactions.	Understand	PSO2
CO9	<i>Differentiate</i> structure and reactions of heterocyclic compounds	Analyze	PSO 6

COURSE CONTENT

Unit 1: Oxidations	8 Hours
<p>1.1. Oxidation of alcohols to carbonyls using DMSO, oxoammonium ions and transition metal oxidants (chromium, manganese, iron, ruthenium).</p> <p>1.2. Epoxydation of alkenes by peroxy acids, Sharpless asymmetric epoxidation, Jacobsen epoxidation, dihydroxylation of alkenes using permanganate ion and osmium tetroxide, Prévost and Woodward dihydroxylations, Sharpless asymmetric dihydroxylation.</p> <p>1.3. Allylic oxidation with CrO₃-Pyridine reagent. Oxidative cleavage of alkenes to carbonyls using O₃.</p> <p>1.4. Oxidative decarboxylation, Riley reaction, Baeyer-Villiger oxidation, Dess-Martin oxidation, Swern oxidation, hydroboration-oxidation.</p>	
Unit 2: Reductions	8 Hours
<p>2.1. Catalytic hydrogenation of alkenes and other functional groups (heterogeneous and homogeneous), Noyori asymmetric hydrogenation, hydrogenolysis.</p> <p>2.2. Liquid ammonia reduction with alkali metals.</p> <p>2.3. Metal hydride reductions. Reduction of carbonyl group with hydrazine, p-tosylhydrazine, diimide and semicarbazide.</p> <p>2.4. Clemmensen reduction, Birch reduction. Wolff-Kishner reduction, Bouveault-Blanc reduction, MPV reduction, hydroboration</p> <p>2.5. Pinacol coupling, McMurry coupling, Shapiro reaction.</p>	
Unit 3: Synthetic Reagents	8 Hours
<p>3.1. Synthetic applications of Crown ethers, β-cyclodextrins, PTC, ionic liquids, Baker's yeast, NBS, LDA, LiAlH₄, LiBH₄, DIEA, BuLi, diborane, 9-BBN, t-butoxycarbonylchloride, DCC, Gilman's reagent, lithium dimethyl cuprate, tri-n-butyltinhydride, 1,3-dithiane, trimethyl silyl chloride, Pb(OAc)₄, ceric ammonium nitrate, DABCO, DMAP, DBU, DDQ, DEAD and Lindlar catalyst in organic synthesis.</p>	

Unit 4: Chemistry of Polymers	8 Hours
<p>4.1. Classification of polymers, chain, step, free-radical and ionic polymerizations. Plastics, rubbers and fibers, thermosets and thermoplastics, linear, branched, cross-linked and network polymers, block and graft copolymers.</p> <p>4.2. Natural and synthetic rubbers.</p> <p>4.3. Biopolymers: Primary, secondary and tertiary structure of proteins</p> <p>4.4. Merrifield solid phase peptide synthesis, Protecting groups, sequence determination of peptides and proteins</p> <p>4.5. Structure and synthesis of glutathione, structure of RNA and DNA, structure of cellulose and starch,</p> <p>4.6. Conversion of cellulose to rayon.</p>	
Unit 5: Heterocyclic chemistry	8 Hours
<p>5.1. Aromatic and nonaromatic heterocyclics. Structure, synthesis and reactions of a few heterocyclics- aziridine, oxirane, pyridine, imidazole.</p> <p>5.2. Structure, synthesis and reactions of fused ring heterocycles: Benzofuran, Indole, Benzothiophene, Quinoline, Benzoxazole, Benzthiazole, Benzimidazole, Triazoles, Oxadiazoles and Tetrazole.</p> <p>5.3. Structure and synthesis of Azepines, Oxepines, Thiepins, Diazepines and Benzodiazepines.</p> <p>5.4. Structure and synthesis (Reichstein process) of Vitamin C (Reichstein process).</p> <p>5.5. Synthesis of uracil, thymine, adenine and guanine</p>	
Unit 6: New reactions in organic synthesis	8 Hours
<p>6.1. Carbon- Carbon double bond forming reactions: Bamford-Stevens reaction, Shapiro reaction, Julia olefination and Peterson olefination.</p> <p>6.2. Ring Formation Reactions: Pauson-Khand reaction, Bergman cyclisation and Nazarov cyclisation, Tiffeneau–Demjanov rearrangement.</p> <p>6.3. Multicomponent Reactions: Biginelli synthesis; multicomponent reactions using alkyl isocyanides–Passerini and Ugi-4-component synthesis.</p> <p>6.4. Olefin metathesis using Grubb’s catalyst.</p>	

6.5. Other important synthetic reactions: Mukaiyama esterification, Mitsunobu reaction and Baylis Hillman reaction.

MODE OF TRANSACTION

Face to Face Instruction: This involves attending traditional classroom lectures and participating in in-person discussions and activities with the instructor and fellow students.

Peer to Peer learning: Students have to select a topic in the course and present it in the class which providing opportunity for critical thinking and feedback.

Group Discussion: Group discussion will be conducted based on the relevant topic in the course that will improve students' thinking and help them to construct their own meaning about academic contents.

MODE OF ASSESSMENT

Internal Assessment (15 Weightage)

- | | |
|---|-------------|
| a. Internal Examination | 2 Weightage |
| <i>2 Internal Examinations, both should be considered</i> | |
| b. Assignments and Exercises: | 3 Weightage |
| c. Seminar/ Viva Voce: | 3 Weightage |
| d. Attendance: | 3 Weightage |

External Assessment (30 Weightages) *Duration 3 Hours, No of Questions: 23*

PATTERN OF QUESTION PAPER

Division	Type	Total No. of questions	No. of questions to be answered	Weightages for each question	Total Weightage
Section A	Short	12	8	1	8
Section B	Short Essay	7	4	3	12

Section C	Essay	4	2	5	10
Total					30

MODULE WISE WEIGHTAGE DISTRIBUTION	
Module	Mark
Unit 1: Oxidations	8
Unit 2: Reductions	9
Unit 3: Synthetic Reagents	9
Unit 4: Chemistry of Polymers	9
Unit 5: Heterocyclic chemistry	9
Unit 6: New reactions in organic synthesis	9
Unit 1: Oxidations	8
Unit 2: Reductions	9

REFERENCES:

1. M. B. Smith, Organic Synthesis, 3/e, Academic Press, 2011.
2. R. O. C. Norman and J. M. Coxon, Principles of Organic Synthesis, 3/e, CRC Press, 1998.
3. W. Carruthers and I. Coldham, Modern Methods of Organic Synthesis, 4/e, Cambridge University Press.
4. R. R. Carey and R. J. Sundburg, Advanced Organic Chemistry, Part B, 5/e, Springer, 2007.
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M.Sc. CHEMISTRY (CBCSS PATTERN)
SEMESTER III

COURSE CODE –MCH3E01 SYNTHETIC ORGANIC CHEMISTRY (ELECTIVE)				
Credit	Hours/week	Weightage		
		Internal	External	Total
4	3	5	30	35

Course Outcomes

CO No.	Expected Course Outcome	Learning Domain	PSO No
	Upon completion of this course, students will be able to;		
CO1	<i>Identify</i> various reagents for oxidation and reduction in organic chemistry	Remember	PSO 1
CO2	<i>Demonstrate</i> the synthetic utility of various reagents organic conversions	Understand	PSO 2 PSO6
CO3	<i>Solve</i> various problems on organic conversions applying various reagents	Apply	PSO 8
CO4	<i>Summarize</i> the key steps in the multistep organic synthesis.	Understand	PSO 2
CO5	<i>Compare</i> the use of different palladium catalyzed reactions in organic synthesis	Analyse	PSO 2 PSO 3
CO6	<i>Apply</i> the concepts of retrosynthetic analysis in synthetic planning of organic compounds	Apply	PSO 11
CO7	<i>Choose</i> the correct reagents for the specific transformations	Create	PSO 9 PSO10
CO8	<i>Summarize</i> classification, structure and synthesis of natural products.	Understand	PSO2

COURSE CONTENT

Unit 1: Reagents for Oxidation and Reduction	8 Hours
<p>1.1. Reagents for oxidation and reduction: Oxone, IBX, PCC, osmium tetroxide, ruthenium tetroxide, selenium dioxide, molecular oxygen (singlet and triplet), peracids, hydrogen peroxide, aluminum isopropoxide, periodic acid, lead tetraacetate.</p> <p>1.2. Wacker oxidation, TEMPO oxidation, Swern oxidation</p> <p>1.3. Woodward and Prevost hydroxylation, Sharpless asymmetric epoxidation.</p> <p>1.4. Catalytic hydrogenations (heterogeneous and homogeneous), metal hydrides, Birch reduction, hydrazine and diimide reduction.</p>	
Unit 2: Organometallic and Organo-nonmetallic Reagents	8 Hours
<p>2.1. Synthetic applications of organometallic and organo-nonmetallic reagents:</p> <p>2.2. Reagents based on chromium, aluminium, nickel, palladium, silicon, and boron, Gilman reagent, phase transfer catalysts, hydroboration reactions, synthetic applications of alkylboranes. Tri-n-butyl tin hydride, Benzene Tricarbonyl Chromium</p>	
Unit 3: Coupling Reactions	8 Hours
<p>3.1. Coupling Reactions: Palladium Catalysts for C-N and C-O bond formation,</p> <p>3.2. Palladium catalyzed amine arylation (Mechanism and Synthetic applications).</p> <p>3.3. Sonogashira cross coupling reaction (Mechanism, Synthetic applications in Cyclic peptides)</p> <p>3.4. Stille carbonylative cross coupling reaction (Mechanism and synthetic applications).</p> <p>3.5. Mechanism and synthetic applications of Negishi, Hiyama, Kumada, Heck and Suzuki-Miyaura coupling reactions.</p>	
Unit 4: Multi step Synthesis	8 Hours

<p>4.1. Multi step Synthesis: Synthetic analysis and planning, Target selection,</p> <p>4.2. Elements of a Synthesis (Reaction methods, reagents, catalysts, solvents, protective groups for hydroxyl, amino, Carbonyl and carboxylic acids, activating groups, leaving groups synthesis and synthetic equivalents.</p> <p>4.3. Types of selectivities (Chemo, regio, stereo selectivities) synthetic planning illustrated by simple molecules, disconnections and functional group interconversions, uplong reactions and use in synthesis,</p>	
Unit 5: Retro Synthetic Analysis	8 Hours
<p>5.1. Retrosynthesis: General principles of retrosynthetic analysis- synthons and reagents, donor and acceptor synthons, umpolung, protecting group chemistry and functional group interconversions.</p> <p>5.2. One group and two group C-X and C-C disconnections, functional group transposition.</p> <p>5.3. Examples for a few retrosynthetic analyses- paracetamol from phenol, benzocain from toluene and propranolol from 1-naphthol. longifolene, Corey lactone, Djerassi Prelog lactone.</p>	
Unit 6: Chemistry of Natural Products	8 Hours
<p>6.1. Chemical classification of natural products. Classification of alkaloids based on ring structure, isolation and general methods of structure elucidation based on degradative reactions.</p> <p>6.2. Structure elucidation of atropine and quinine.</p> <p>6.3. Terpenoids - Isolation and classification of terpenoids, structure of steroids classification of steroids.</p> <p>6.4. Woodward synthesis of cholesterol, conversion of cholesterol to testosterone. Total synthesis of Reserpine, Cephalosporin,</p> <p>6.5. General structure of anthocyanins and flavonoids.</p>	

MODE OF TRANSACTION

Module	Mark
Unit 1: Reagents for Oxidation and Reduction	8
Unit 2: Organometallic and Organo non-metallic Reagents	9
Unit 3: Coupling Reactions	9
Unit 4: Multi step Synthesis	9
Unit 4: Multi step Synthesis	9
Unit 6: Chemistry of Natural Products	9

REFERENCES:

1. M. B. Smith, Organic Synthesis, 3/e, Academic Press, 2011.
2. S. Warren and P. Wyatt, Organic Synthesis: Strategy and Control, John Wiley
3. S. Warren: Organic Synthesis: The Disconnection Approach, John Wiley
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5. W. Carruthers and I. Coldham, Modern Methods of Organic Synthesis, 4/e, Cambridge University Press.
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M.Sc. CHEMISTRY (CBCSS PATTERN)
SEMESTER III

COURSE CODE –MCH3E02 COMPUTATIONAL CHEMISTRY (ELECTIVE)				
Credit	Hours/week	Weightage		
		Internal	External	Total
4	3	5	30	35

Course Outcomes

CO No.	Expected Course Outcome	Learning Domain	PSO No
	Upon completion of this course, students will be able to;		
CO1	<i>Develop</i> working knowledge of terminology and tools used by quantum chemists	Understand	PSO 8
CO2	<i>Analyse</i> how quantum mechanics manifests itself in nature and experimental science	Evaluate	PSO 3
CO3	<i>Summarize</i> advanced quantum mechanical method	Remember	PSO 1
CO4	<i>Understand</i> the basics of computational chemistry	Understand	PSO 8
CO5	<i>Illustrate</i> various tools of computational chemistry	Analyse	PSO 2 PSO 3
CO6	<i>Evaluate</i> the types of chemical problems and suitability of advanced quantum chemical methods.	Evaluate	PSO 3 PSO 10
CO7	<i>Apply</i> computational chemistry as an alternative and complements to the experimental methods in chemistry	Apply	PSO 7

COURSE CONTENT

Unit 1: Introduction to Computational Chemistry	8 Hours
<p>1.1. Theory, computation & modeling – Definition of terms; Need of approximate methods in quantum mechanics.</p> <p>1.2. Computable Quantities – structure, potential energy surfaces and chemical properties.</p> <p>1.3. Cost & Efficiency – relative CPU time, software & hardware; Classification of computational methods</p>	
Unit 2: Computer Simulation Methods- I	8 Hours
<p>2.1. Introduction – molecular dynamics and Monte Carlo methods, calculation of simple thermodynamic properties - energy, heat capacity, pressure and temperature, phase space, practical aspects of computer simulation, periodic boundary conditions.</p> <p>2.2. Monitoring the equilibration, analyzing the results of a simulation, error estimation.</p>	
Unit 3: Computer Simulation Methods- II	8 Hours
<p>3.1. Molecular dynamics (MD) method – molecular dynamics using simple models.</p> <p>3.2. MD with continuous potentials, finite difference methods, choosing the time step, setting up and running a MD simulation.</p> <p>3.3. Monte Carlo (MC) method - calculating properties by integration, Metropolis method, random number generators, MC simulation of rigid molecules.</p>	
Unit 4: ab initio Methods in Computational Chemistry	8 Hours
<p>4.1. Review of Hartree – Fock method for atoms, SCF treatment of polyatomic molecules; Closed shell systems - restricted HF calculations</p> <p>4.2. Open shell systems – ROHF and UHF calculations.</p> <p>4.3. The Roothan – Hall equations, Koopmans theorem, HF limit & electron correlation,</p>	

4.4. Introduction to electron correlation (post -HF) methods.	
Unit 5: Density Functional Methods	8 Hours
<p>5.1. Introduction to density matrices, N-repeatability & V-representability problems. Hohenberg – Kohn theorems, Kohn-Sham orbitals</p> <p>5.2. Exchange correlation functionals – Thomas-Fermi-Dirac model, Local density approximation.</p> <p>5.3. Generalized gradient approximation, hybrid functionals; Comparison between DFT and HF methods.</p>	
Unit 6: Basis Set Approximation	8 Hours
<p>6.1. Hydrogen-like, Slater-type & Gaussian type basis functions</p> <p>6.2. Classification of basis sets – minimal, double zeta, triple zeta, split-valence, polarization & diffuse basis sets, even tempered & well tempered basis sets, contracted basis sets</p> <p>6.3. Pople-style basis sets and their nomenclature, correlation consistent basis sets, basis set truncation error, effect of choice of method/ basis set (model chemistries) on CPU time.</p>	

MODE OF TRANSACTION
<p>Face to Face Instruction: This involves attending traditional classroom lectures and participating in in-person discussions and activities with the instructor and fellow students.</p> <p>Peer to Peer learning: Students have to select a topic in the course and present it in the class which providing opportunity for critical thinking and feedback.</p> <p>Group Discussion: Group discussion will be conducted based on the relevant topic in the course that will improve students’ thinking and help them to construct their own meaning about academic contents.</p>

MODE OF ASSESSMENT					
Internal Assessment (15 Weightage)					
a. Internal Examination		2 Weightage			
<i>2 Internal Examinations, both should be considered</i>					
b. Assignments and Exercises:		3 Weightage			
c. Seminar/ Viva Voce:		3 Weightage			
d. Attendance:		3 Weightage			
External Assessment (30 Weightages) <i>Duration 3 Hours, No of Questions: 23</i>					
PATTERN OF QUESTION PAPER					
Division	Type	Total No. of questions	No. of questions to be answered	Weightages for each question	Total Weightage
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Section C	Essay	4	2	5	10
Total					30

MODULE WISE WEIGHTAGE DISTRIBUTION	
Module	Mark
Unit 1: Introduction to Computational Chemistry	8
Unit 2: Computer Simulation Methods- I Error! Reference source	9
Unit 3: Computer Simulation Methods- II	9
Unit 4: ab initio Methods in Computational Chemistry	9
Unit 5: Density Functional Methods	9
Unit 6: Basis Set Approximation	9

REFERENCES:

1. C. J. Cramer, Essentials of computational Chemistry: Theories and models, John Wiley & Sons 2002.
2. Frank Jensen, Introduction to Computational Chemistry, John Wiley & Sons LTD 1999.
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M.Sc. CHEMISTRY (CBCSS PATTERN)
SEMESTER III

COURSE CODE –MCH3E03				
GREEN CHEMISTRY AND NANOCHEMISTRY (ELECTIVE)				
Credit	Hours/week	Weightage		
		Internal	External	Total
4	3	5	30	35

Course Outcomes

CO No.	Expected Course Outcome	Learning Domain	PSO No
	Upon completion of this course, students will be able to;		
CO1	Describe twelve principles of green chemistry	Remember	PSO 1 PSO 2
CO2	Design environment friendly chemical reactions based on green chemistry principles	Create	PSO9 PSO10
CO3	Demonstrate different types of microwave mediated organic synthesis	Understand	PSO2
CO4	Choose alternative synthesis, reagents and reaction conditions for different applications	Apply	PSO9 PSO11
CO5	Demonstrate physicochemical methods for the synthesis of diverse types of nanomaterials	Understand	PSO2
CO6	Explain working principles and analysis of nanomaterials based on different instruments	Create	PSO4 PSO 11
CO7	Compare different microscopic techniques	Evaluate	PSO6
CO8	Distinguish carbon nanostructures in terms of structural, optical and electrical properties	Analyse	PSO6
CO9	Design new techniques to prepare various nanomaterials for environmental applications	Create	PSO10 PSO11

COURSE CONTENT

Unit 1: Introduction to green chemistry	8 Hours
<p>1.1. Green chemistry-relevance and goals,</p> <p>1.2. Anastas' twelve principles of green chemistry</p> <p>1.3. Tools of green chemistry: alternative starting materials, reagents, catalysts, solvents and processes with suitable examples.</p>	
Unit 2: Microwave mediated organic synthesis (MAOS)	Hours
<p>2.1. Microwave activation –advantage of microwave exposure – specific effects of microwave</p> <p>2.2. Neat reactions – solid supports reactions- Functional group transformations – condensations reactions- oxidations – reductions reactions – multi-component reactions.</p>	
Unit 3: Alternative synthesis, reagents and reaction conditions	8 Hours
<p>3.1. Introduction – synthesis of ionic liquids – physical properties – applications in alkylation – hydroformylations – epoxidations</p> <p>3.2. Synthesis of ethers – Friedel-craft reactions – Diels-Alder reactions – Knoevengal condensations – Wittig reactions</p> <p>3.3. Phase transfer catalyst - Synthesis – applications.</p> <p>3.4. Photochemical alternative to Friedel-crafts reactions</p> <p>3.5. Dimethyl carbonate as a methylating agent</p> <p>3.6. The design and applications of green oxidants</p> <p>3.7. Super critical carbon dioxide for synthetic chemistry.</p>	
Unit 4: Nanomaterials – An Introduction & Synthetic Methods	8 Hours
<p>4.1. Definition of nano dimensional materials - Historical milestones - unique properties due to nanosize,Quantum dots.</p> <p>4.2. Classification of Nanomaterials</p> <p>4.3. General methods of synthesis of nanomaterials – Hydrothermal synthesis, Solvothermal synthesis, Microwave irradiation, sol – gel and Precipitation technologies, Combustion Flame-Chemical Vapor Condensation Process, gas</p>	

<p>Phase Condensation Synthesis, Reverse Micelle Synthesis, Polymer – Mediated Synthesis, Protein Microtube – Mediated Synthesis Synthesis of Nanomaterials using microorganisms and other biological agents, Sonochemical Synthesis, Hydrodynamic Cavitation.</p> <p>4.4. Inorganic nanomaterials – Typical examples – nano TiO₂ / ZnO/CdO/CdS.</p> <p>4.5. Organic nanomaterials – examples – Rotaxanes and Catenanes</p>	
<p>Unit 5: Techniques for Characterisation of nanoscale materials</p>	<p>8 Hours</p>
<p>5.1. Principles of Atomic force microscopy (AFM)</p> <p>5.2. Transmission electron microscopy (TEM)</p> <p>5.3. Resolution and scanning transition electron microscopy (STEM)</p> <p>5.4. Scanning Tunneling Microscopy (STM)</p> <p>5.5. Scanning nearfield optical microscopy (SNOM) - Scanning ion conductance microscope, scanning thermal microscope, scanning probe microscopes and surface plasmon spectroscopy.</p>	
<p>Unit 6: Carbon Clusters and Nanostructures</p>	<p>8 Hours</p>
<p>6.1. Nature of carbon bond - new carbon structures - Carbon clusters: Discovery of C₆₀ - Alkali doped C₆₀ -Superconductivity in C₆₀ - Larger and smaller fullerenes.</p> <p>6.2. Carbon nanotubes: Synthesis - Single walled carbon nanotubes - Structure and characterization - Mechanism of formation - Chemically modified carbon nanotubes - Doping - Functionalizing nanotubes - Application of carbon nanotubes.</p> <p>6.3. Nanowires - Synthetic strategies - Gas phase and solution phase growth - Growth control - Properties.</p>	

<p>MODE OF TRANSACTION</p>
<p>Face to Face Instruction: This involves attending traditional classroom lectures and participating in in-person discussions and activities with the instructor and fellow students.</p>

Peer to Peer learning: Students have to select a topic in the course and present it in the class which providing opportunity for critical thinking and feedback.

Group Discussion: Group discussion will be conducted based on the relevant topic in the course that will improve students' thinking and help them to construct their own meaning about academic contents.

MODE OF ASSESSMENT

Internal Assessment (15 Weightage)

- | | |
|---|-------------|
| a. Internal Examination | 2 Weightage |
| <i>2 Internal Examinations, both should be considered</i> | |
| b. Assignments and Exercises: | 3 Weightage |
| c. Seminar/ Viva Voce: | 3 Weightage |
| d. Attendance: | 3 Weightage |

External Assessment (30 Weightages) *Duration 3 Hours, No of Questions: 23*

PATTERN OF QUESTION PAPER

Division	Type	Total No. of questions	No. of questions to be answered	Weightages for each question	Total Weightage
Section A	Short	12	8	1	8
Section B	Short Essay	7	4	3	12
Section C	Essay	4	2	5	10
Total					30

MODULE WISE WEIGHTAGE DISTRIBUTION

Module	Mark
Unit I: Introduction to green chemistry	8
Unit-2: Microwave mediated organic synthesis (MAOS)	9

Unit 3: Alternative synthesis, reagents and reaction conditions	9
Unit 4: Nanomaterials – An Introduction & Synthetic Methods	9
Unit 5: Techniques for Characterisation of nanoscale materials	9
Unit 6: Carbon Clusters and Nanostructures	9

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1. V. K. Ahluwalia, Green Chemistry – Environmentally benign reactions, Ane Books India (Publisher), (2006).
2. V. K. Ahluwalia, Green Chemistry: A Textbook, Narosa Publishing House, 2013.
3. Green Chemistry – Designing Chemistry for the Environment – edited by Paul T. Anastas & Tracy C. Williamson. Second Edition, (1998).
4. Green Chemistry – Frontiers in benign chemical synthesis and processes- edited by Paul T. Anastas & Tracy C. Williamson. Oxford University Press, (1998).
5. Green Chemistry – Environment friendly alternatives- edited by Rashmi Sanghi & M. M. Srivastava, Narora Publishing House, (2003).
6. C.N.R. Rao, A. Muller, A.K. Cheetam (Eds), The Chemistry of Nanomaterials, Vol.1, 2, Wiley –VCH, Weinheim, 2004.
7. C.P. Poole, Jr: F.J. Owens, Introduction to Nanotechnology Wiley Interscience, New Jersey, 2003
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11. Bengt Nolting, Methods in modern biophysics, Springer-Verlag, Berlin, First Indian Reprint, 2004. (Pages 102-146 for Unit II and 147 – 163 for Unit V)
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17. Home page of Prof. Ned Seeman - <http://seemanlab4.chem.nyu.edu/>
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19. Nanotation - <http://www.acsnanotation.org/>

M.Sc. CHEMISTRY (CBCSS PATTERN)
SEMESTER IV

COURSE CODE –MCH4C12				
INSTRUMENTAL METHODS OF ANALYSIS				
Credit	Hours/week	Weightage		
		Internal	External	Total
4	4	5	30	35

Course Outcomes

CO No.	Expected Course Outcome	Learning Domain	PSO No
	Upon completion of this course, students will be able to;		
CO1	<i>Identify</i> types of errors.	Remember	PSO 1 PSO 2
CO2	<i>Compare</i> analytical methods	Evaluate	PSO 3
CO3	<i>Summarize</i> mechanism of precipitation	Understand	PSO 8
CO4	<i>Illustrate</i> various electrodes	Analyse	PSO 2 PSO 3
CO5	<i>Distinguish</i> Emission and absorption analysis instruments	Analyse	PSO 3
CO6	<i>Classify</i> different polarographic techniques	Understand	PSO 1
CO7	<i>Distinguish</i> different thermal analysis instruments	Analyse	PSO 3
CO8	<i>Judge</i> choice of suitable detectors.	Evaluate	PSO 3 PSO 10
CO9	<i>Differentiate</i> types of chromatographic techniques	Analyze	PSO 6
CO10	<i>Compare</i> different microscopic techniques	Evaluate	PSO 3

COURSE CONTENT

Unit 1: Errors in Chemical Analysis	8 Hours
<p>1.1. Treatment of analytical data, accuracy and precision, Absolute and relative errors</p> <p>1.2. Classification and minimization of errors, significant figures,</p> <p>1.3. Statistical treatment- mean and standard deviation, variance, confidence limits, student-t and f tests, detection of gross errors, rejection of a result-Q test.</p> <p>1.4. Least square method, linear regression; covariance and correlation coefficient</p>	
Unit 2: Conventional Analytical Procedures	8 Hours
<p>2.1. Gravimetry: solubility product and properties of precipitates-nucleation, growth and aging, co- precipitation and post precipitation, drying and ignition. Inorganic precipitating agents: NH_3, H_2S, H_2SO_4, $(\text{NH}_4)_2\text{MoO}_4$ and NH_4SCN.</p> <p>2.2. Organic precipitating agents: oxine, cupron, cupferron, 1-nitroso-Inaphthol, dithiocarbamates, Acid-Base and precipitation titrations: theory of neutralisation titrations, indicators for acid/base titrations, titration curves of strong acid, strong base, weak acid, weak base and polyprotic acids. Buffer solutions.</p> <p>2.3. Titrations in nonaqueous media. Different solvents and their selection for a titration. Indicators for non-aqueous titrations</p> <p>2.4. Redox titrations: Permanganometry, dichrometry, iodometry, cerimetry. Variation of potential during a redox titration, formal potential during a redox titration, Redox indicators.</p> <p>2.5. Precipitation titrations, adsorption indicators</p> <p>2.6. Complexometric titrations: Types of EDTA titrations (direct, back, replacement, alkalimetric and exchange reactions), masking and demasking agents, selective demasking, metal ion indicators - murexide, eriochrome black T, Patton and Reeder's indicators, bromopyrogallol red, xylenol orange, variamine blue.</p>	
Unit 3: Electro Analytical Methods- I	8 Hours

<p>3.1. Potentiometry: techniques based on potential measurements, direct potentiometric systems, different types of indicator electrodes, limitations of glass electrode, applications in pH measurements, modern modifications, other types of ion selective electrodes, solid, liquid, gas sensing and specific types of electrodes, biomembrane, biological and biocatalytic electrodes as biosensors, importance of selectivity coefficients.</p> <p>3.2. Polarography micro electrode and their specialities, potential and current variations at the micro electrode systems, conventional techniques for concentration determination, limitations of detection at lower concentrations,</p> <p>3.3. Techniques of improving detection limit-rapid scan, ac, pulse, differential pulse square wave polarographic techniques.</p> <p>3.4. Applications of polarography.</p>	
<p>Unit 4: Electro Analytical Methods II</p>	<p>8 Hours</p>
<p>4.1. Amperometry: biamperometry, amperometric titrations.</p> <p>4.2. Coulometry-primary and secondary coulometry, advantages of coulometric titrations, applications. Principle of chronopotentiometry.</p> <p>4.3. Anodic stripping voltammetry-different types of electrodes and improvements of lower detection limits. Voltammetric sensors.</p> <p>4.4. Organic polarography.</p>	
<p>Unit 5: Optical Methods - I</p>	<p>8 Hours</p>
<p>5.1. Fundamental laws of spectrophotometry, nephelometry and turbidometry and fluorimetry.</p> <p>5.2. UV- visible and IR spectrophotometry – instrumentation, single and double beam instruments, Spectrophotometric titrations.</p> <p>5.3. Atomic emission spectrometry – excitation sources (flame, AC and DC arc), spark, inductively coupled plasma, glow discharge, laser microprobes, flame structure, instrumentation, and qualitative and quantitative analysis.</p> <p>5.4. Atomic absorption spectrometry: sample atomization techniques, instrumentation, interferences, background correction, and analytical applications.</p>	

Unit 6: Optical Methods - II	8 Hours
<p>6.1. Theory, instrumentation, and applications of: - Atomic fluorescence spectrometry</p> <p>6.2. X-ray methods, X-ray absorption and X-ray diffraction, photoelectron spectroscopy, Auger, ESCA.</p> <p>6.3. SEM, TEM, AFM.</p>	
Unit 7: Thermal Methods	8 Hours
<p>7.1. Thermogravimetry (TG), Differential Thermal Analysis (DTA) and Differential Scanning Calorimetry (DSC)</p> <p>7.2. Thermomechanical Analysis (TMA), Dynamic Mechanical Analysis (DMA), and their instrumentation. Thermometric Titrations.</p>	
Unit 8: Chromatography	8 Hours
<p>8.1. Chromatography-classification-column-paper and thin layer chromatography. HPLC-outline study of instrument modules. Ion – exchange chromatography-Theory.</p> <p>8.2. Important applications of chromatographic techniques. Gel Permeation Chromatography.</p> <p>8.3. Gas chromatography – basic instrumental set up-carriers, columns, detectors and comparative study of TCD, FID, ECD and NPD. Qualitative and quantitative studies using GC</p> <p>8.4. Preparation of GC columns, selection of stationary phases of GLC, Gas adsorption chromatography, applications, CHN analysis by GC</p>	

MODE OF TRANSACTION
<p>Face to Face Instruction: This involves attending traditional classroom lectures and participating in in-person discussions and activities with the instructor and fellow students.</p>

Peer to Peer learning: Students have to select a topic in the course and present it in the class which providing opportunity for critical thinking and feedback.

Group Discussion: Group discussion will be conducted based on the relevant topic in the course that will improve students' thinking and help them to construct their own meaning about academic contents.

MODE OF ASSESSMENT

Internal Assessment (15 Weightage)

- | | |
|---|-------------|
| a. Internal Examination | 2 Weightage |
| <i>2 Internal Examinations, both should be considered</i> | |
| b. Assignments and Exercises: | 3 Weightage |
| c. Seminar/ Viva Voce: | 3 Weightage |
| d. Attendance: | 3 Weightage |

External Assessment (30 Weightages) *Duration 3 Hours, No of Questions: 23*

PATTERN OF QUESTION PAPER

Division	Type	Total No. of questions	No. of questions to be answered	Weightages for each question	Total Weightage
Section A	Short	12	8	1	8
Section B	Short Essay	7	4	3	12
Section C	Essay	4	2	5	10
Total					30

MODULE WISE WEIGHTAGE DISTRIBUTION

Module	Mark
Unit 1: Errors in Chemical Analysis	6
Unit 2: Conventional Analytical Procedures	6

Unit 3: Electro Analytical Methods- I	6
Unit 4: Electro Analytical Methods II	7
Unit 5: Optical Methods - I	7
Unit 6: Optical Methods - II	7
Unit 7: Thermal Methods	7
Unit 8: Chromatography	7

REFERENCES:

1. J.M. Mermet, M. Otto, R. Kellner, Analytical Chemistry, Wiley-VCH, 2004.
2. D.A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, Fundamentals of Analytical Chemistry, 9th Edn., Cengage Learning., 2014.
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M.Sc. CHEMISTRY (CBCSS PATTERN)
SEMESTER III & IV

COURSE CODE –MCH3L07 & MCH4L10				
INORGANIC CHEMISTRY PRACTICALS– III & IV				
Credit	Hours/week	Weightage		
		Internal	External	Total
3	4*	10	30	40

* 4 hours/week in semester III and 3 hours/week in semester IV

Course Outcomes

CO. No	Expected Course Outcome	Learning Domain	PSO No.
	Upon completion of this course, students will be able to;		
CO1	Recognize methods to separate different ions	Remember	PSO 1 PSO 2
CO2	Compare different separation methods and chose the best	Evaluate	PSO 3 PSO 4 PSO 10
CO3	Develop quantitative skills	Analyse	PSO 3 PSO 5 PSO 6 PSO 11
CO4	Determine the quantity of different ions in a mixture	Evaluate	PSO 4 PSO 10
CO5	Explain choice of solvents for separation	Apply	PSO 3 PSO 10
CO6	Prepare inorganic complexes	Apply	PSO 4 PSO 10 PSO 11
CO7	Assess Purity and yield of synthesised complexes	Evaluate	PSO 2 PSO 11

COURSE CONTENT

Experiment	112 Hours
Unit 1: Estimation of ions in mixture	
1.1. Estimation involving quantitative separation of suitable binary mixtures of ions in solution (Cu^{2+} , Ni^{2+} , Zn^{2+} , Fe^{2+} , Ca^{2+} , Mg^{2+} , Ba^{2+} and $\text{Cr}_2\text{O}_7^{2-}$) by volumetric colorimetric or gravimetric methods only one of the components to be estimated	
Unit 2: Colorimetric Estimations	
2.1. Colorimetric estimations of Ni, Cu, Fe and Mo, after separation from other ions in solution by solvent extraction. (Minimum two experiments.)	
Unit 3: Ion Exchange Methods	
3.1. Ion- exchange separation and estimation of binary mixtures (Co^{2+} & Ni^{2+} , Zn^{2+} and Mg^{2+} . Hardness of water).	
Unit 4: Preparation of Inorganic Complexes (5 Nos)	

Mode of Transaction
<p>Demonstrations: Helps to illustrate and consolidate theoretical principles outlined in the course.</p> <p>Experimentation: This involves learning by doing or hands on experience by applying chemical principles.</p> <p>Observation: It involves noticing or perceiving the course of the experiment or measurement by equipment and acquisition of information from the primary source:</p>

Mode of Assessment	
Internal Assessment (10 Weightage)	
f. Attendance:	2 weightage
g. Lab skill/quality of their results:	2 weightage
h. Model practical test:	2 weightage
<i>(Best one, out of two model exams is considered)</i>	
i. Record:	2 weightage
j. Viva Voce:	2 weightage
External Assessment (30 Weightage)	

SEE will be at the end of the fourth semester.

REFERENCES:

1. Vogel's Textbook of Qualitative Inorganic Analysis.
2. IM. Kolthoff and E. A. Sanderson, Quantitative Chemical Analysis.
3. D. A. Adams and J. B. Rayner, Advanced Practical Inorganic Chemistry.
4. W. G. Palmer, Experimental Inorganic Chemistry.
5. G. Brauer, Handbook of Preparative Inorganic Chemistry.

M.Sc. CHEMISTRY (CBCSS PATTERN)
SEMESTER III & IV

COURSE CODE –MCH3L08 & MCH4L11 ORGANIC CHEMISTRY PRACTICALS– III & IV				
Credit	Hours/week	Weightage		
		Internal	External	Total
3	4*	10	30	40

* 4 hours/week in semester III and 3 hours/week in semester IV

Course Outcomes

CO No.	Expected Course Outcome	Learning Domain	PSO No.
	Upon completion of this course, students will be able to;		
CO1	<i>Recognize</i> different methods to estimate various organic molecules and drugs	Remember	PSO 1 PSO 2
CO2	<i>Compare</i> different extraction methods used for separation of natural products	Evaluate	PSO 3 PSO 4 PSO 10
CO3	<i>Develop</i> quantitative skills	Analyse	PSO 5 PSO 6 PSO 11
CO4	<i>Determine</i> the quantity of organic compounds present.	Evaluate	PSO 4 PSO 10
CO5	<i>Develop</i> methods for chromatographic separations of natural products, Food colours, food additives and dyes.	Create	PSO 10
CO6	<i>Identify</i> suitable separations methods for organic compounds	Analyze	PSO 5 PSO 8
CO7	<i>Assess</i> Purity drugs and organic compounds	Evaluate	PSO 2 PSO 11

COURSE CONTENT

Experiment	112 Hours
Unit 1: Quantitative Organic Analysis	
1.1. Estimation of equivalent weight of acids by Silver Salt method 1.2. Estimation of nitrogen by Kjeldahl method 1.3. Determination of Acid value, iodine value and saponification value of oils and fats (at least one each) 1.4. Estimation of reducing sugars, Estimation of amino group, phenolic group and esters. 1.5. Colourimetric estimations: Vitamins (Ascorbic acid), Drugs – sulphadiazine, sulphathiazole, Antibiotics – Penicillin, Streptomycin.	
Unit 2: Extractions	
2.1. Extraction of Natural products and purification by column chromatography and TLC – Caffeine from Tea waste, Chlorophyll Steroids, Flavonoid (Soxhlet extraction), citral from lemon grass (steam distillation). 2.2. Casein from milk	
Unit 3: Chromatography	
3.1. Food additives and Dyes, Artificial sweeteners: Saccharine, cyclamates, Dulcin. Flavour adulterants – piperonal, Benzalacetate, ethyl acetate antioxidants: Butylated hydroxytoluene (BHT) Butylated hydroxy anisole (BHA), Hydroquinone. 3.2. Food colours: Permitted – Amaranth, Erythrosine, Tartrazine, sunset yellow, Fast green, Brilliant Blue, Nonpermitted colours: Auramine, Congo red, Malachite green, Metanil yellow, Orange II, Sudan II, Congo red. 3.3. Amino acids (Protein hydrolysates), Sugars, Terpenoids, Alkaloids, Flavonoids, Steroids. Pesticides and herbicides: Organochlorine pesticides organophosphates and carbamate pesticides, Herbicides. 3.4. Plant growth stimulants: Indole acetic acid.	

Mode of Transaction

Demonstrations: Helps to illustrate and consolidate theoretical principles outlined in the course.

Experimentation: This involves learning by doing or hands on experience by applying chemical principles.

Observation: It involves noticing or perceiving the course of the experiment or measurement by equipment and acquisition of information from the primary source:

Mode of Assessment

Internal Assessment (10 Weightage)

- | | |
|---|-------------|
| k. Attendance: | 2 weightage |
| l. Lab skill/quality of their results: | 2 weightage |
| m. Model practical test: | 2 weightage |
| <i>(Best one, out of two model exams is considered)</i> | |
| n. Record: | 2 weightage |
| o. Viva Voce: | 2 weightage |

External Assessment (30 Weightage)

SEE will be at the end of the fourth semester.

REFERENCES:

1. B.S. Furnis, A.J. Hannaford, P.W.G. Smith and A.R. Tatchell, Vogel's Textbook of Practical Organic Chemistry, 5/e, Pearson, 1989.
2. Beebet, Pharmacuetical Analysis
3. E. Hoftmann, Chromatography, Nostrand Reinhold Company, New York, 1975.
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5. H. Wagner, S. Bladt, E.M. Zgainsti – Tram, Th. A. Scott., Plant Drug Analysis, Springer- Verlag, Tokyo, 1984.
6. Vishnoi, Practical Organic Chemistry.

M.Sc. CHEMISTRY (CBCSS PATTERN)
SEMESTER III & IV

COURSE CODE –MCH3L09 &MCH4L12				
PHYSICAL CHEMISTRY PRACTICALS– III & IV				
Credit	Hours/week	Weightage		
		Internal	External	Total
3	4*	10	30	40

* 4 hours/week in semester III and 3 hours/week in semester IV

Course Outcomes

CO No	Expected Course Outcome	Learning Domain	PSO No.
	Upon completion of this course, students will be able to;		
CO1	Recognize methods for studying physical properties of molecules and materials	Remember	PSO 1 PSO 2
CO2	Compare the physical properties of molecules and materials	Evaluate	PSO 3 PSO 4 PSO 10
CO3	Develop skills for analyzing physical properties of materials	Analyse	PSO 3 PSO 6 PSO 11
CO4	Determine the physical parameters	Evaluate	PSO 4 PSO 10
CO5	Explain the factors affecting the various physical properties of compounds	Apply	PSO 3 PSO 10
CO6	Design experiments for studying physical properties of compound and reactions	Create	PSO 9 PSO 10 PSO 11
CO7	Assess the basic molecular parameters of simple molecules using computational softwares	Evaluate	PSO 2 PSO 11

COURSE CONTENT

Experiment	112 Hours
Unit 1: Chemical Kinetics (4 experiments)	
1.1. Determination of specific reaction rate of acid hydrolysis of an ester (methyl acetate or ethyl acetate) and concentration of the given acids. 1.2. Determination of Arrhenius parameters of acid hydrolysis of an ester 1.3. Determination of specific reaction rate of saponification of ethyl acetate 1.4. Iodination of acetone in acid medium – Determination of order of reaction with respect of iodine and acetone.	
Unit 2: Adsorption (3 experiments)	
2.1. Verification of Langmuir adsorption isotherm – charcoal-acetic acid system. 2.2. Determination of the concentration of a given acetic acid solution using the isotherm 2.3. Verification of Langmuir adsorption isotherm – charcoal-oxalic acid system. 2.4. Determination of the concentration of a given acetic acid solution using the isotherm. 2.5. Determination of surface area of adsorbent	
Unit 3: Phase Equilibria (2 experiments)	
3.1. Determination of phase diagram of a ternary liquid system (eg. chloroform–acetic acid – water – Benzene – acetic acid –water) 3.2. Determination of the composition of a binary liquid mixture (e.g., chloroform-acetic acid, benzene-acetic acid) 3.3. Determination of mutual miscibility curve of a binary liquid system (e.g., phenol –water) and critical solution temperature(CST). 3.4. Effect of impurities (e.g, NaCl, KCl, succinic acid, salicylic acid) on the CST of water-phenol system 3.5. Effect of a given impurity (e.g., KCl) on the CST of water –phenol system and determination of the concentration of the given solution	

Unit 4: Cryoscopy – Beckman Thermometer (3 experiments)
<p>4.1. Determination of cryoscopic constant of a liquid (water, benzene)</p> <p>4.2. Determination of molecular mass of a solute (urea, glucose, cane sugar, mannitol) by studying the depression in freezing point of a liquid solvent (water, benzene)</p> <p>4.3. Determination of Van't Hoff factor and percentage of dissociation of NaCl.</p> <p>4.4. Study of the reaction $2KI + HgI_2 \rightleftharpoons K_2HgI_4$ and determination of the concentration of the given KI solution.</p>
Unit 5: Polarimetry (3 experiments)
<p>5.1. Determination of specific and molar optical rotations of glucose, fructose and sucrose.</p> <p>5.2. Determination of specific rate of inversion of cane sugar in presence of HCl.</p> <p>5.3. Determination of concentration of HCl</p>
Unit 6: Spectrophotometry (3 experiments)
<p>6.1. Determination of equilibrium constants of acid –base indicators.</p> <p>6.2. Simultaneous determination of Mn and Cr in a solution of $KMnO_4$ and $K_2Cr_2O_7$</p> <p>6.3. Investigation of complex formation between Fe (III) and thiocyanate</p>
Unit 7: Computational Chemistry Calculations
<p>7.1. Single point energy calculations of simple molecules like H_2O and NH_3 at the HF/3-21G level of theory.</p> <p>7.2. The effect of basis set on the single point energy of H_2O and NH_3 using the</p> <p>7.3. Hartree-Fock method (3-21G, 6-31G, 6-31+G, 6-31+G* basis sets can be used).</p> <p>7.4. Geometry optimization of molecules like H_2O, NH_3, HCHO & C_2H_4 at the HF/6-31G level of theory.</p> <p>7.5. Computation of dipole and quadrupole moments of HCHO & C_2H_4 at the HF/6-31G level of theory.</p>

- 7.6. Effect of basis set on the computation of H-O-H bond angle in H₂O using the Hartree-Fock method (3-21G, 6-31G, 6-31+G, 6-31+G* basis sets can be used).
- 7.7. Computation of the energy of HOMO and LUMO of formaldehyde and ethylene at the HF/6-31G level of theory.
- 7.8. Effect of substituent (F & Cl) on the geometric parameters (like C-C bond length) of ethylene at the HF/6-31G level of theory.
- 7.9. Comparison of stability of cis-planar and trans-planar conformers of H₂O₂ at the HF/6-31G level of theory.
- 7.10. Comparison of stability of cis- and trans- isomers of difluoroethylene at the HF/6-31G* level of theory.
- 7.11. Computation of the frequencies of normal modes of vibration of molecules like H₂O, NH₃ and CO₂ at the HF/6-31+G* level of theory.
- 7.12. Determination of hydrogen bond strength of H₂O dimer and H₂O trimer at the HF/6-31+G* level of theory.
- 7.13. Determination of hydrogen bond strength of HF dimer and HF trimer at the HF/6-31+G* level of theory.

Mode of Transaction

Demonstrations: Helps to illustrate and consolidate theoretical principles outlined in the course.

Experimentation: This involves learning by doing or hands on experience by applying chemical principles.

Observation: It involves noticing or perceiving the course of the experiment or measurement by equipment and acquisition of information from the primary source:

Mode of Assessment	
Internal Assessment (10 Weightage)	
p. Attendance:	2 weightage
q. Lab skill/quality of their results:	2 weightage
r. Model practical test:	2 weightage
<i>(Best one, out of two model exams is considered)</i>	
s. Record:	2 weightage
t. Viva Voce:	2 weightage
External Assessment (30 Weightage)	

SEE will be at the end of the fourth semester.

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6. J.B. Yadav, Advanced Practical Physical Chemistry, Goel Publications, 1989.
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M.Sc. CHEMISTRY (CBCSS PATTERN)
SEMESTER IV

COURSE CODE –MCH4E04				
PETROCHEMICALS AND COSMETICS (ELECTIVE)				
Credit	Hours/week	Weightage		
		Internal	External	Total
4	4	5	30	35

Course Outcomes

CO No.	Expected Course Outcome	Learning Domain	PSO No
	Upon completion of this course, students will be able to;		
CO1	<i>Understand</i> the basics of petroleum refining	Remember	PSO 1 PSO 2
CO2	<i>Identify</i> the raw materials obtained from petroleum	Analyse	PSO3
CO3	<i>Classify</i> Chemical processing of various hydrocarbons	Remember	PSO 1 PSO 2
CO4	<i>Understand</i> the processes in industrial organic synthesis	Understand	PSO 1
CO5	<i>Analyse</i> Physical Properties and Test Methods	Analyse	PSO 2 PSO 3
CO6	<i>Evaluate</i> Physical Properties	Evaluate	PSO 3 PSO 10
CO7	<i>Understand</i> the basics of distillation of crude oil	Remember	PSO 1 PSO 2
CO8	<i>Discuss</i> the products of distillation of crude oil	Remember	PSO 1 PSO 2

COURSE CONTENT

Unit 1: Introduction to Petrochemistry	8 Hours
<p>1.1. Introduction – Petroleum – Refining of crude oil – Fuels for internal combustion engines. Knocking, Octane number. Unleaded petrol.</p> <p>1.2. Diesel Engine and Cetane number. Cracking – Thermal, Catalytic. Mechanism of cracking process. Reforming Activation Gasoline. Petrochemicals.</p>	
Unit 2: Hydrocarbons from Petroleum	8 Hours
<p>2.1. Introduction. Raw materials. Saturated hydrocarbons from natural gas. Uses of saturated hydrocarbons. Unsaturated hydrocarbons – Acetylene, Ethylene, Propylene, Butylenes.</p> <p>2.2. Aromatic hydrocarbons - Benzene. Toluene. Xylenes. Chemical processing of paraffin hydrocarbons. Chemical processing of ethylene hydrocarbons. Chemical processing of acetylene. Chemical processing of aromatic hydrocarbons.</p>	
Unit 3: Industrial Organic Synthesis	8 Hours
<p>3.1. Introduction. The raw materials and basic processes.</p> <p>3.2. Chemical process used in industrial organic synthesis. Petrochemicals- Methanol. Important points. Ethanol. Important points.</p> <p>3.3. Rectified spirit from beer. Methylated spirit. Proof spirit. Preparation of the absolute alcohol from rectified spirit. Acetaldehyde. Acetic acid. Isopropanol. Ethylene glycol. Glycerine. Acetone. Phenol. Formaldehyde. Important points. Ethyl acetate. Important points.</p>	
Unit 4: Composition of Petroleum Crude	8 Hours
<p>4.1. Composition of petroleum crude. Composition of the petroleum products. Isomeric compounds. Classification of petroleum crude. A survey of the world crude. Sulphur compounds in petroleum.</p> <p>4.2. Physical Properties and Test Methods</p> <p>4.3. Viscosity: Other methods for finding out viscosity. Viscosity of an oil blend. Use of the figure for finding out viscosity. Viscosities of hydrocarbons. 2.</p>	

<p>Density, 3. Surface and interfacial tensions. 4. Refractive Index. 5. Flash and fire points. 6. Cloud and pour points. 7. Aniline point. 8. Diesel index. 9. Cetane number. 10. Octane number and knock characteristics. 11. Distillation curves. (a) ASTM (American Society for Testing Materials) distillation curve. (b). Hempel or semi fractionating distillation curve.</p>	
<p>Unit 5: Distillation of Crude Petroleum</p>	<p>8 Hours</p>
<p>5.1. Preparation of petroleum for processing. Destruction of petroleum emulsion. Electric desalting plants.</p> <p>5.2. Fundamentals of preliminary distillation. Methods of petroleum distillation. Distillation of crude petroleum. Treatment of the residual liquid processing of liquid fuels such as petroleum and petroleum products.</p> <p>5.3. Petroleum processing equipments. Storage tanks. Rectification columns. Cap tray or bubble tray columns. Heat exchange apparatus. Steam space heaters or boilers. Condensers. Pipe furnaces. Pipelines. Fitting Compressors and pumps.</p>	
<p>Unit 6: Petroleum Products</p>	<p>8 Hours</p>
<p>6.1. Introduction. Classification of petroleum products. Liquefied hydrocarbons, gases and fuels. Fuel oils or boiler oils. Fuel for Jet engines and gas turbine engines.</p> <p>6.2. Lubricants, products of oil paraffine processing and other petroleum products.</p> <p>6.3. Lubricating and other oils. Paraffins, ceresins, petroleum. Miscellaneous petroleum products.</p> <p>6.4. Products of petrochemical and basic organic synthesis. Dye intermediates. Lacquers. Solvents. Thinners.</p>	
<p>Unit 7: Purification of Petroleum Products</p>	<p>8 Hours</p>
<p>7.1. Absorptive and adsorptive purification. Sulphuric acid purification. Alkaline purification. Hydrorefining.</p> <p>7.2. Purification in a DC electric field. New methods of purification. De mercaptanisation. Stabilisation.</p>	
<p>Unit 8: Perfumes and Cosmetics</p>	<p>8 Hours</p>

- 8.1. Perfumes: Introduction. Esters. Alcohols. Ketones. Ionones. Nitromusks. Aldehydes. Diphenyl compounds. Production of natural perfumes. Flower perfume. Fruit flavours. Artificial flavours.
- 8.2. Cosmetics: Introduction. Toothpaste. Ingredients. Preparation. Recipe for toothpaste. Shampoos. Ingredients. Recipe. Hair dyeing. Materials used. Colour and Curl of Hair. Creams and Lotions. Skin Chemicals. Their ingredients. Preparation and recipe. Lipsticks. Ingredients. Preparation and recipe. Perfumes, Colognes and after shave preparation.
- 8.3. Compounds with flowery and fruity odours used in perfumes with their structures. Compounds with unpleasant odours used to fix delicate odours in perfumes. Deodorants and Antiperspirants.
- 8.4. Cosmetics: Economics and Advertising.

MODE OF TRANSACTION

Face to Face Instruction: This involves attending traditional classroom lectures and participating in in-person discussions and activities with the instructor and fellow students.

Peer to Peer learning: Students have to select a topic in the course and present it in the class which providing opportunity for critical thinking and feedback.

Group Discussion: Group discussion will be conducted based on the relevant topic in the course that will improve students' thinking and help them to construct their own meaning about academic contents.

MODE OF ASSESSMENT

Internal Assessment (15 Weightage)

- a. Internal Examination 2 Weightage
2 Internal Examinations, both should be considered
- b. Assignments and Exercises: 3 Weightage

c. Seminar/ Viva Voce:	3 Weightage				
d. Attendance:	3 Weightage				
External Assessment (30 Weightages)	<i>Duration 3 Hours, No of Questions: 23</i>				
PATTERN OF QUESTION PAPER					
Division	Type	Total No. of questions	No. of questions to be answered	Weightages for each question	Total Weightage
Section A	Short	12	8	1	8
Section B	Short Essay	7	4	3	12
Section C	Essay	4	2	5	10
Total					30

MODULE WISE WEIGHTAGE DISTRIBUTION	
Module	Mark
Unit 1: Introduction to Petrochemistry	4
Unit 2: Hydrocarbons from Petroleum	4
Unit 3: Industrial Organic Synthesis	9
Unit 4: Composition of Petroleum Crude	9
Unit 5: Distillation of Crude Petroleum	9
Unit 6: Petroleum Products	9
Unit 7: Purification of Petroleum Products	4
Unit 8: Perfumes and Cosmetics	5

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3. John W. Hill, Chemistry for Changing times, Surjeet Publication
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5. S ukumar Maiti, "Introduction To Petrochemicals" India Book House Pvt Ltd.
6. Gabriella Baki, Kenneth S. Alexander, "Introduction to Cosmetic Formulation and Technology", Wiley.
7. Tony Curtis, David Williams, "Introduction to Perfumery", Micelle Press; 2nd edition

M.Sc. CHEMISTRY (CBCSS PATTERN)
SEMESTER IV

COURSE CODE –MCH4E05 INDUSTRIAL CATALYSIS (ELECTIVE)				
Credit	Hours/week	Weightage		
		Internal	External	Total
4	4	5	30	35

Course Outcomes

CO No.	Expected Course Outcome	Learning Domain	PSO No
	Upon completion of this course, students will be able to;		
CO1	<i>Understand</i> adsorption processes	Remember	PSO 1 PSO 2
CO2	<i>Distinguish</i> adsorption processes	Analyse	PSO3
CO3	<i>Evaluate</i> surface area of materials	Analyse	PSO3 PSO5
CO4	<i>Understand</i> various theories of adsorption processes	Remember	PSO 1 PSO 2
CO5	<i>Apply</i> various theories in adsorption to solve problems in kinetics	Apply	PSO8
CO6	<i>Understand</i> industrial importance of catalysts	Remember	PSO 1 PSO 2
CO7	<i>Solve</i> problems in surface chemistry	Apply	PSO8
CO8	<i>Acquire</i> knowledge regarding various synthetic methods for preparing catalysts	Remember	PSO 1 PSO 2
CO9	<i>Recognize</i> various techniques used for surface analyses	Remember	PSO1 PSO11

COURSE CONTENT

Unit 1: Introduction To Adsorption Process	8 Hours
<p>1.1. Intermolecular interactions, physisorption – the forces of adsorption – dispersion and repulsive forces – classical electrostatic interactions – adsorbate-adsorbate interactions, chemisorption, potential energy curves,</p> <p>1.2. Thermodynamics of adsorption – isothermal and adiabatic heats of adsorption – variation of heats of adsorption with coverage</p> <p>1.3. Adsorption isotherms, Langmuir, BET and Freundlich,</p> <p>1.4. Kinetics of chemisorption – activated and non-activated chemisorption – absolute rate theory – electronic theories, hysteresis, and shapes of capillaries.</p>	
Unit 2: Kinetics And Catalysis	8 Hours
<p>2.1. Adsorption and catalysis – adsorption and reaction rate – strength of adsorption bond and catalysis – adsorption equilibrium and catalysis,</p> <p>2.2. Kinetics of heterogeneous catalysis: diffusion steps neglected – unimolecular reactions – bimolecular reactions – Langmuir-Hinshelwood and Eley-Rideal mechanism,</p> <p>2.3. Kinetics of heterogeneous catalysis: diffusion controlling – mechanism of diffusion – diffusion and reaction in pores – selectivity and diffusion, electronic factors in catalysis by metals, electronic factors in catalysis by semiconductors, geometric factors and catalysis.</p>	
Unit 3: Catalyst - Preparative Methods	8 Hours
<p>3.1. Surface area and porosity measurement – measurement of acidity of surfaces; Support materials</p> <p>3.2. Preparation and structure of supports – surface properties, preparation of catalysts – introduction of precursor compound – pre-activation treatment – activation process.</p> <p>3.3. General methods of synthesis of zeolites, mechanism of nuclear formation and crystal growth, structures of some selected zeolites – zeolites A, X and Y, pentasils – ZSM-5, ZSM-11, shape selective catalysis by zeolites.</p>	

Unit 4: Deactivation Of Catalysts	8 Hours
<p>4.1. Deactivation of catalysts, classification of catalyst deactivation processes, poisoning of catalysts, coke formation on catalysts, metal deposition on catalysts, sintering of catalysts,</p> <p>4.2. Regeneration of deactivated catalysts, feasibility of regeneration, description of coke deposit and kinetics of regeneration.</p>	
Unit 5: Phase Transfer Catalysis	8 Hours
<p>5.1. Basic concepts in phase transfer catalysis – phase transfer catalyzed reactions – basic steps of phase transfer catalysis – effect of reaction variables on transfer and intrinsic rates – outline of compounds used as phase transfer catalysts.</p> <p>5.2. Use of quaternary salts – macrocyclic and macrobicyclic ligands – PEG's and related compounds</p> <p>5.3. Use of dual phase transfer catalyst or co-catalyst in phase transfer systems – separation and recovery of phase transfer catalysts.</p> <p>5.4. Insoluble phase transfer catalysts.</p>	
Unit 6: Biocatalysis	8 Hours
<p>6.1. Enzymes – an introduction to enzymes – enzymes as proteins</p> <p>6.2. Classification and nomenclature of enzymes</p> <p>6.3. Structure of enzymes – how enzymes work – effect on reaction rate – thermodynamic definitions – catalytic power and specificity of enzymes – optimization of weak interactions between enzyme and substrate in the transition state – binding energy, reaction specificity and catalysis – specific catalytic groups contributing to catalysis.</p> <p>6.4. Immobilized biocatalysts – definition and classification of immobilized biocatalysts – immobilization of coenzymes</p>	
Unit 7: Industrial Catalysis-1	8 Hours

<i>2 Internal Examinations, both should be considered</i>					
b. Assignments and Exercises:		3 Weightage			
c. Seminar/ Viva Voce:		3 Weightage			
d. Attendance:		3 Weightage			
External Assessment (30 Weightages) <i>Duration 3 Hours, No of Questions: 23</i>					
PATTERN OF QUESTION PAPER					
Division	Type	Total No. of questions	No. of questions to be answered	Weightages for each question	Total Weightage
Section A	Short	12	8	1	8
Section B	Short Essay	7	4	3	12
Section C	Essay	4	2	5	10
Total					30

MODULE WISE WEIGHTAGE DISTRIBUTION	
Module	Mark
Unit 1: Introduction to Adsorption process	6
Unit 2: Kinetics and Catalysis	6
Unit 3: Catalyst - Preparative Methods	6
Unit 4: Deactivation of Catalysts	7
Unit 5: Phase Transfer Catalysis	7
Unit 6: Biocatalysis	7
Unit 7: Industrial Catalysis-I	7
Unit 8: Industrial Catalysis-II	7

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1. A Clark, "Theory of adsorption and catalysis", Academic Press, 1970.
2. J.M. Thomas & W.J. Thomas, "Introduction to principles of heterogeneous catalysis",

3. Academic Press, New York, 1967.
4. R.H.P. Gasser, "An introduction to chemisorption and catalysis by metals", Oxford, 1985.
5. D.K Chakraborty, "Adsorption and catalysis by solids", Wiley Eastern Ltd. 1990.
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7. R.B. Anderson, "Experimental methods in catalysis research", Vol I, II, Academic press, NY, 1981.
8. R. Szostak, "Molecular sieves: principles of synthesis and identification", Van Nostrand, NY, 1989.
9. R. Hughes, "Deactivation of catalysts", Academic press, London, 1984.
10. C.M. Starks, C.L. Liotta And M. Halpern, "Phase Transfer Catalysis – Fundamentals, Applications And Industrial Perspectives", Chapman & Hall, New York, 1994.
11. A.L. Lehninger, "Principles of Biochemistry", Worth Publishers, USA, 1987.
12. G. Ertl, H. Knozinger and J. Weitkamp, "Handbook of Heterogeneous Catalysis" Vol 1-5, Wiley-VCH, Weinheim, 1997.
13. R.J. Farrauto and C.H. Bartholomew, "Fundamentals of Industrial Catalytic Processes", Blackie Academic and Professional – Chapman and Hall, 1997.
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M.Sc. CHEMISTRY (CBCSS PATTERN)
SEMESTER IV

COURSE CODE –MCH4E06				
NATURAL PRODUCTS & POLYMER CHEMISTRY (ELECTIVE)				
Credit	Hours/week	Weightage		
		Internal	External	Total
4	4	5	30	35

Course Outcomes

CO No.	Expected Course Outcome	Learning Domain	PSO No
	Upon completion of this course, students will be able to;		
CO1	Classify different types of natural products	Understand	PSO 1 PSO 2
CO2	Explain isolation and constituents of different essential oils	Apply	PSO4 PSO9
CO3	Demonstrate structural elucidation of terpenoids and alkaloids	Understand	PSO1 PSO2
CO4	Classify alkaloids and anthocyanins	Analyse	PSO2
CO5	Categorize different dyes and pigments	Analyse	PSO2
CO6	Interrelate different polymerization processes	Understand	PSO1
CO7	Distinguish chemistry of different types of polymerisations.	Analyse	PSO4
CO8	Explain Polymerization techniques	Create	PSO4
CO9	Describe the properties and uses of different industrial polymers	Remember	PSO9
CO10	Design new polymers with remarkable optical, electrical and mechanical properties	Create	PSO10

COURSE CONTENT

Unit 1: Basic aspects of Natural Products	8 Hours
<p>1.1. Classification of Natural Products: Classification of Natural products based on chemical structure, physiological activity, taxonomy and Biogenesis.</p> <p>1.2. Carbohydrates, Terpenoids, Carotenoids, alkaloids, steroids, anthocyanins etc. Methods of isolation of each class of compound</p> <p>1.3. Essential Oils: Isolation and study of important constituents of lemon grass oil, citronella oil, cinnamon oil, palmarosa oil, turpentine oil, clove oil, sandalwood oil, Essential oils of turmeric and ginger.</p> <p>1.4. Oleoresins of pepper, chilly, ginger and turmeric. Aromatherapy.</p>	
Unit 2: Terpenoids and Steroids	8 Hours
<p>2.1. Terpenoids: classification, structure elucidation and synthesis of abietic acid.</p> <p>2.2. Steroids: Classification - structure of Cholesterol, Ergosterol, Oesterone, Androsterone, Testosterone, Progesterone, Cortisone and Corticosterone. Structural elucidation of Cholesterol. Conversion of cholesterol to progesterone, androsterone and testosterone.</p> <p>2.3. Classification, structure and synthesis of prostaglandins, biosynthesis of fatty acids, prostaglandins, terpenoids and steroids.</p>	
Unit 3: Alkaloids and Anthocyanins	8 Hours
<p>3.1. Alkaloids – classification of alkaloids, structure elucidation based on degradative reactions (quinine and atropine). Biosynthesis of quinine and papaverine.</p> <p>3.2. Anthocyanins: Introduction, General Nature and Structure of Anthocyanidins. Flavone, Flavonol, Isoflavone and Chalcone</p>	
Unit 4: Dyes, Pigments and Supramolecules	8 Hours
<p>4.1. Brief introduction to dyes and pigments (natural and synthetic): b-carotene, indigo, cyclic tetrapyrroles (porphyrins, chlorins, chlorophyll, heme), study of phthalocyanines, squarenes, cyanine dyes.</p>	

4.2. Introduction to Supramolecular chemistry and Molecular Recognition	
Unit 5: Polymerization Processes	8 Hours
<p>5.1. Polymerization processes. Free radical addition polymerization. Kinetics and mechanism. Chain transfer. Mayo-walling equation of the steady state. Molecular weight distribution and molecular weight control. Radical Atom Transfer and Fragmentation – Addition mechanism. Free radical living polymers.</p> <p>5.2. Cationic and anionic polymerization. Kinetics and mechanism, Polymerization without termination. Living polymers. Step Growth polymerization. Kinetics and mechanism. Molecular weight distribution. Linear Vs cyclic polymerization, other modes of polymerization.</p> <p>5.3. Group Transfer, metathesis and ring opening polymerization. Copolymerization. The copolymerization equation, Q-e scheme,</p> <p>5.4. Gelation and Crosslinking.</p> <p>5.5. Copolymer composition drift Polymerization techniques. Bulk Solution, melt, suspension, emulsion and dispersion techniques.</p>	
Unit 6: Characterization and Stereochemistry of Polymers	8 Hours
<p>6.1. Polymer Stereochemistry. Organizational features of polymer chains. Configuration and conformation, Tacticity, Repeating units with more than one asymmetric centre.</p> <p>6.2. Chiral polymers – main chain and side chain. Stereoregular polymers. Manipulation of polymerization processes. Zeigler-Natta and Kaminsky routes.</p> <p>6.3. Coordination polymerization. Metallocene and Metal oxide catalysts.</p> <p>6.4. Polymer Characterization. Molecular weights. Concept of average molecular weights, Molecular weight distribution. Methods for determining molecular weights. Static and dynamic methods, Light scattering and GPC.</p> <p>6.5. Crystalline and amorphous states. Glassy and Rubbery States. Glass transition and crystalline melting. Spherulites and Lammellac. Degree of Crystallinity, X-ray diffraction</p>	

Unit 7: Polymer Solutions, Industrial polymers and Copolymers	8 Hours
<p>7.1. Polymer Solutions. Treatment of dilute solution data. Thermodynamics. Flory-Huggins equation.</p> <p>7.2. Chain dimension-chain stiffness – End-to-end distance. Conformation-random coil, Solvation and Swelling. Flory-Reiner equation.</p> <p>7.3. Determination of degree of crosslinking and molecular weight between crosslinks.</p> <p>7.4. Industrial polymers. Synthesis, Structure and applications. Polyethylene, polypropylene, polystyrene.</p> <p>7.5. Homo and Copolymers. Diene rubbers. Vinyl and acrylic polymers. PVC, PVA, PAN, PA. PMMA and related polymers.</p> <p>7.6. Copolymers. EVA polymers. Fluorine containing polymers. Polyacetals. Reaction polymers. Polyamides, polyesters. Epoxides, polyurethanes, polycarbonates, phenolics, PEEK, Silicone polymers.</p>	
Unit 8: Speciality Polymers	8 Hours
<p>8.1. Reactions of polymers. Polymers as aids in Organic Synthesis. Polymeric Reagents, Catalysts, Substrates.</p> <p>8.2. Liquid Crystalline polymers. Main chain and side chain liquid crystalline polymers. Phase morphology.</p> <p>8.3. Conducting polymers. Polymers with high bandwidth. Polyanilines, polypyrrols, polythiophenes, poly(vinylene phenylene).</p> <p>8.4. Photoresponsive and photorefractive polymers. Polymers in optical lithography. Polymer photoresists.</p> <p>8.5. Electrical properties of Polymers, Polymers with NLO properties, second and third harmonic generation, wave guide devices.</p>	

MODE OF TRANSACTION

Unit 1: Basic aspects of Natural Products	6
Unit 2: Terpenoids and Steroids	7
Unit 3: Alkaloids and Anthocyanins	6
Unit 4: Dyes, Pigments and Supramolecules	7
Unit 5: Polymerization processes	7
Unit 6: Characterization and Stereochemistry of Polymers	7
Unit 7: Polymer Solutions, Industrial polymers and Copolymers	7
Unit 8: Speciality polymers	6

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1. M. B. Smith, Organic Synthesis, 3/e, Academic Press, 2011.
2. F. A. Carey and R. J. Sundberg: Advanced Organic Chemistry (part B), 3rd ed., Plenum Press.
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M.Sc. CHEMISTRY (CBCSS PATTERN)
SEMESTER IV

COURSE CODE –MCH4E07				
MATERIAL SCIENCE (ELECTIVE)				
Credit	Hours/week	Weightage		
		Internal	External	Total
4	4	5	30	35

Course Outcomes

CO No.	Expected Course Outcome	Learning Domain	PSO No
	Upon completion of this course, students will be able to;		
CO1	<i>Understand</i> various materials and their properties	Remember	PSO 1 PSO 2
CO2	<i>Categorize</i> various materials	Analyse	PSO3
CO3	<i>Evaluate</i> mechanical properties of materials	Analyse	PSO3 PSO5
CO4	<i>Understand</i> nanomaterials and their preparation	Remember	PSO 1 PSO 2
CO5	<i>Identify</i> materials for special purpose	Analyse	PSO3
CO6	<i>Understand</i> fundamental theories and properties of magnetic materials	Remember	PSO 1 PSO 2
CO7	<i>Acquire</i> knowledge regarding various synthetic methods for preparing catalysts	Apply	PSO8

COURSE CONTENT

Unit 1: Introduction to Material Science	8 Hours
<p>1.1. Introduction, classification of materials, functional classification, classification based on structure, environmental and other effects, material design and selection.</p> <p>1.2. Mechanical properties – significance and terminology, the tensile test, true stress and true strain, bend test, hardness of materials.</p>	
Unit 2: Ceramic Materials	8 Hours
<p>2.1. Definition of ceramics, traditional and new ceramics, structure of ceramics, atomic interactions and types of bonds</p> <p>2.2. Phase equilibria in ceramic systems, one component and multi component systems, use of phase diagrams in predicting material behaviour, electrical, magnetic, and optical properties of ceramic materials.</p>	
Unit 3: Nanomaterials and Nanotechnology	8 Hours
<p>3.1. Nanomaterials, nanostructures, self-assembly, Nanoparticles- methods of synthesis, sol-gel process, hydrolysis of salts and alkoxides, precipitation, condensation reactions, electrokinetic potential and peptization reactions;</p> <p>3.2. Gelatin network- xerogels, aerogels, drying of gels</p> <p>3.3. Chemical modifications of nanosurfaces, applications of sol-gel process, sol-gel coating, porous solids, catalysts, dispersions and powders</p>	
Unit 4: Materials for Special Purposes – I	8 Hours
<p>4.1. Production of ultra pure materials - zone refining, vacuum distillation and electro refining</p> <p>4.2. Ferroelectric and piezoelectric materials - general properties, classification of ferroelectric materials, theory of ferroelectricity, ferroelectric domains, applications, piezoelectric materials and applications</p> <p>4.3. Metallic glasses - preparation, properties and applications.</p>	
Unit 5: Materials for Special Purposes – II	8 Hours

<p>5.1. Magnetic materials, ferri and ferro magnetism, metallic magnets, soft, hard & superconducting magnets</p> <p>5.2. Ceramic magnets, low conducting and superconducting magnets;</p> <p>5.3. Superconducting materials - metallic and ceramic superconducting materials, theories of superconductivity</p> <p>5.4. Meissner effect; High temperature superconductors - structure and applications</p>	
Unit 6: Some Special Polymers	8 Hours
<p>6.1. Functional polymers - photoconductive, electroconductive, piezoelectric and light sensitive polymers.</p> <p>6.2. Industrial polymers - production, properties, & compounding of industrial polymers.</p> <p>6.3. Commodity plastics such as PP, PE, PVC, & PS</p> <p>6.4. Engineering plastics such as polyacetyl, polyamide (nylon 6 and nylon 66), polyacrylate, polycarbonate, polyester (PET, PBT), polyether ketones;</p> <p>6.5. Thermosetting plastics such as PF, UF & MF</p>	
Unit 7: Composite Materials	8 Hours
<p>7.1. Definition and classification of composites, fibres and matrices; Composites with metallic matrices – processing, solid and liquid state processing, deposition.</p> <p>7.2. Ceramic matrix composite materials – processing, mixing & pressing, liquid state processing, sol -gel processing & vapor deposition technique; Interfaces in composites - mechanical & microstructural characteristics.</p> <p>7.3. Applications of composites.</p>	
Unit 8: Fracture Mechanics	8 Hours
<p>8.1. Importance of fracture mechanics, micro structural features of fracture in metals, ceramics, glasses & composites, Weibull statistics for failure, strength analysis.</p>	

8.2. Fatigue, application of fatigue testing - creep, stress rupture & stress behaviour, evaluation of creep behaviour.

MODE OF TRANSACTION

Face to Face Instruction: This involves attending traditional classroom lectures and participating in in-person discussions and activities with the instructor and fellow students.

Peer to Peer learning: Students have to select a topic in the course and present it in the class which providing opportunity for critical thinking and feedback.

Group Discussion: Group discussion will be conducted based on the relevant topic in the course that will improve students' thinking and help them to construct their own meaning about academic contents.

MODE OF ASSESSMENT

Internal Assessment (15 Weightage)

- | | |
|---|-------------|
| a. Internal Examination | 2 Weightage |
| <i>2 Internal Examinations, both should be considered</i> | |
| b. Assignments and Exercises: | 3 Weightage |
| c. Seminar/ Viva Voce: | 3 Weightage |
| d. Attendance: | 3 Weightage |

External Assessment (30 Weightages) *Duration 3 Hours, No of Questions: 23*

PATTERN OF QUESTION PAPER

Division	Type	Total No. of questions	No. of questions to be answered	Weightages for each question	Total Weightage
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Section A	Short	12	8	1	8
Section B	Short Essay	7	4	3	12
Section C	Essay	4	2	5	10
Total					30

MODULE WISE WEIGHTAGE DISTRIBUTION	
Module	Mark
Unit 1: Introduction to Material Science	6
Unit 2: Ceramic Materials	6
Unit 3: Nanomaterials and Nanotechnology	6
Unit 4: Materials for Special Purposes – I	7
Unit 5: Materials for Special Purposes – II	7
Unit 6: Some Special Polymers	7
Unit 7: Composite Materials	7
Unit 8: Fracture Mechanics	7

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M.Sc. CHEMISTRY (CBCSS PATTERN)
SEMESTER IV

COURSE CODE –MCH4E08				
ORGANOMETALLIC CHEMISTRY (ELECTIVE)				
Credit	Hours/week	Weightage		
		Internal	External	Total
4	4	5	30	35

Course Outcomes

CO No.	Expected Course Outcome	Learning Domain	PSO No
	Upon completion of this course, students will be able to;		
CO1	<i>Understand</i> the basics of Organometallic compounds and their properties	Remember	PSO 1 PSO 2
CO2	<i>Categorize</i> Organometallic compounds	Analyse	PSO3
CO3	<i>Evaluate</i> the properties of organometallic compounds	Analyse	PSO3 PSO5
CO4	<i>Understand</i> bonding in organometallic compounds	Remember	PSO 1 PSO 2
CO5	<i>Identify</i> the methods of synthesis of different organometallic compounds	Analyse	PSO3
CO6	<i>Understand</i> fundamental theories and properties of organometallic compounds	Remember	PSO 1 PSO 2
CO7	<i>Acquire</i> knowledge regarding various reactions and applications of organometallic compounds	Apply	PSO8
CO8	<i>Illustrate</i> the catalytic activity of organometallic compounds	Apply	PSO3 PSO8

COURSE CONTENT

Unit 1: Introduction to organometallic compounds	8 Hours
<p>1.1. Organometallic compounds, Classification and nomenclature, the 16 and 18 electron rules, electron counting-covalent and ionic models</p> <p>1.2. Main group organometallics-alkyl and aryl, groups 1, 2, 12, 13, 14 and 15 synthesis structure and applications.</p> <p>1.3. Transition metal to carbon multiple bond-the metal carbenes and carbynes,</p> <p>1.4. Transition metal complexes with chain π ligands – synthesis, structure, bonding and reactions of complexes of ethylene, allyl, butadiene and acetylene.</p>	
Unit 2: Metal carbonyls and their reactions	8 Hours
<p>2.1. Metal carbonyls- Bonding modes of CO, IR spectroscopy as a tool to study bonding and structure of metal carbonyls, Synthesis of Metal carbonyls Direct and reductive Carbonylation.</p> <p>2.2. Reactions of Metal carbonyls-Activation of metal carbonyls, Disproportion, Nucleophilic addition, electrophilic addition to the carbonyl oxygen,</p> <p>2.3. Carbonyl cation, anions and hydrides, Collmann's reagent, Migratory insertion of carbonyls, Oxidative decarbonylation,</p> <p>2.4. Photochemical substitution, Microwave assisted substitution.</p>	
Unit 3: Main group organometallic compounds, metal carbenes and carbynes	8 Hours
<p>3.1. General aspects of synthesis, structure, reactivity and applications of main group organometallic compounds. Metal complexes of NO, H₂, CS, RNC and Phosphines.</p> <p>3.2. Metal-carbon multiple bonds - Metal carbenes and carbynes, bridging carbenes and carbynes, N-heterocyclic carbons, multiple bonds to hetero atoms.</p>	
Unit 4: Organometallic π complexes	8 Hours

<p>4.1. Organometallic π complexes – synthesis, structure, bonding (molecular orbital treatment) and reactions of C_5H_5, C_6H_6, C_7H_7 and $C_8H_8^{-2}$.</p> <p>4.2. Polyalkyls, polyhydrides and f-block organometallic complexes, Fluxional organometallics.</p>	
Unit 5: Organometallic compounds in catalysis	8 Hours
<p>5.1. Applications of organometallic compounds in organic synthesis and homogeneous catalysis, Complex formation and activation of H_2, N_2, O_2, NO by transition metals. Catalytic steps, Oxidative addition, reductive elimination and insertion reactions Hydrozirconation of alkenes and alkynes.</p> <p>5.2. Homogeneous catalysis. Hydrogenation, isomerization of alkenes, alkyne, cycloadditions, Zeigler-Natta catalysis, hydroformylation of alkenes, Monsanto acetic acid process and Wacker process.</p> <p>5.3. Metal complexes in enantioselective synthesis</p>	
Unit 6: Organometallic reactions	8 Hours
<p>6.1. Organometallic reactions. SN_2 Reactions, Radical Mechanisms, Ionic Mechanisms, σ-Bond Metathesis, Oxidative</p> <p>6.2. Coupling and Reductive decoupling, Reactions involving CO, Insertions Involving Alkenes, Other Insertions, α, β, γ and δ Elimination,</p> <p>6.3. Deinsertion and Nucleophilic and electrophilic attack on coordinated ligand.</p>	
Unit 7: Applications of organometallic reaction	8 Hours
<p>7.1. Applications of organometallic reaction- Homogeneous catalysis- General features of catalysis, Types of catalyst, Catalytic steps.</p> <p>7.2. Water-gas shift reaction, Fisher-Tropsch reaction, Hydrosilation of alkenes, Hydrocyanation of alkenes.</p>	
Unit 8: Organometallic Polymers	8 Hours
<p>8.1. Organometallic Polymers, Polymers with organometallic moieties as pendant groups, polymers with organometallic moieties in the main chain</p>	

8.2. Condensation polymers based on ferrocene and on rigid rod polyynes, poly(ferrocenylsilane)s, applications of poly(ferrocenylsilane)s and related polymers.

8.3. Applications of rigid-rod polyynes, polygermanes and polystannanes, polymers prepared by ring opening polymerization, organometallic dendrimers

MODE OF TRANSACTION

Face to Face Instruction: This involves attending traditional classroom lectures and participating in in-person discussions and activities with the instructor and fellow students.

Peer to Peer learning: Students have to select a topic in the course and present it in the class which providing opportunity for critical thinking and feedback.

Group Discussion: Group discussion will be conducted based on the relevant topic in the course that will improve students' thinking and help them to construct their own meaning about academic contents.

MODE OF ASSESSMENT

Internal Assessment (15 Weightage)

- | | |
|---|-------------|
| a. Internal Examination | 2 Weightage |
| <i>2 Internal Examinations, both should be considered</i> | |
| b. Assignments and Exercises: | 3 Weightage |
| c. Seminar/ Viva Voce: | 3 Weightage |
| d. Attendance: | 3 Weightage |

External Assessment (30 Weightages) *Duration 3 Hours, No of Questions: 23*

PATTERN OF QUESTION PAPER

Division	Type	Total No. of questions	No. of questions to be answered	Weightages for each question	Total Weightage
Section A	Short	12	8	1	8
Section B	Short Essay	7	4	3	12
Section C	Essay	4	2	5	10
Total					30

MODULE WISE WEIGHTAGE DISTRIBUTION	
Module	Mark
Unit 1: Introduction to organometallic compounds	6
Unit 2: Metal carbonyls and their reactions	6
Unit 3: Main group organometallic compounds, metal carbenes and	6
Unit 4: Organometallic π complexes	7
Unit 5: Organometallic compounds in catalysis	7
Unit 6: Organometallic reactions	7
Unit 7: Applications of organometallic reaction	7
Unit 8: Organometallic Polymers	7

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M.Sc. CHEMISTRY (CBCSS PATTERN)
SEMESTER IV

COURSE CODE –MCH4E09 ADVANCED TOPICS IN CHEMISTRY (ELECTIVE)				
Credit	Hours/week	Weightage		
		Internal	External	Total
4	4	5	30	35

Course Outcomes

CO No.	Expected Course Outcome	Learning Domain	PSO No
	Upon completion of this course, students will be able to;		
CO1	<i>Identify</i> supramolecular interactions.	Remember	PSO 1 PSO 2
CO2	<i>Compare</i> Energy sources	Evaluate	PSO 3
CO3	<i>Summarize</i> organic semiconductors and electronics	Understand	PSO 8
CO4	<i>Illustrate</i> various characterisation techniques of nanomaterials	Analyse	PSO 2 PSO 3
CO5	<i>Distinguish</i> synthesis approaches to nanomaterials	Analyse	PSO 3
CO6	<i>Classify</i> drugs	Understand	PSO 1
CO7	<i>Distinguish</i> internal coordinates and cartesian coordinates	Analyse	PSO 3
CO8	<i>Judge</i> choice of basis sets	Evaluate	PSO 3 PSO 10
CO9	<i>Compare</i> different types of catalysis	Evaluate	PSO 3

COURSE CONTENT

Unit 1: : Chemistry of Nanomaterials	16 Hours
<p>1.1. History of Nanomaterials - Classification. Size- dependence of properties. Electronic structure theory of metals and semiconductors. Quantum size effects.</p> <p>1.2. Synthesis of nanostructures: bottom-up-approach, top - down approach, self assembly, lithography techniques – photolithography, soft lithography, dip-pen nanolithography.</p> <p>1.3. Introduction to carbon nanomaterials.</p> <p>1.4. Characterizations of Nanomaterials: UV-Visible spectroscopy, Photoluminescence spectroscopy, Raman Spectroscopy, Dynamic light scattering (DLS), X-ray diffraction (XRD), Energy Dispersive X-ray analysis (EDAX), X-ray photoelectron spectroscopy (XPS),</p> <p>1.5. Electron microscopic techniques - SEM, TEM. Scanning probe microscopies - STM, AFM – Scanning tunneling spectroscopy</p> <p>1.6. Measurement of electrical properties of nanomaterials.</p> <p>1.7. Applications: Nanoelectronics, nanosensors, nanocatalysts, nanofiltration, diagnostic and therapeutic applications and targeted drug delivery.</p>	
Unit 2: Introduction to computational quantum chemistry	8 Hours
<p>2.1. Electronic structure of molecules-Review of Hartree-Fock SCF method.</p> <p>2.2. Basis sets STOs and GTOs . Nomenclature of Basis sets. Semi empirical and ab initio methods.</p> <p>2.3. Calculations using Gaussian programme . Specification of molecular geometry using a) Cartesian coordinates and b) Internal coordinates.</p> <p>2.4. The Z-matrix . Z- matrices of some simple molecules like H₂,H₂O, formaldehyde ammonia and methanol.</p>	
Unit 3: Supramolecular Chemistry	8 Hours
<p>3.1. Concepts and language. Molecular recognition: Molecular receptors for different types of molecules, design and synthesis of coreceptors and multiple recognition.</p>	

<p>3.2. Host-guest systems – Crown ether, cryptants, podants, calixarenes, Cucurbituril.</p> <p>3.3. Supramolecular Strong, weak and very weak Hydrogen bonds. Utilisation of H-bonds to create supramolecular structures. Use of H bonds in crystal engineering and molecular recognition. Supramolecular reactivity and catalysis.</p> <p>3.4. Transport processes and carrier design.</p> <p>3.5. Supramolecular devices. Supramolecular photochemistry, supramolecular electronic, ionic and switching devices some examples of self- assembly in supramolecular chemistry</p>	
<p>Unit 4: Medicinal Chemistry</p>	<p>8 Hours</p>
<p>4.1. Drugs: Introduction, different classes of drug, drug action, drug design, pro drugs, factors governing drug design, rational approach to drug design.</p> <p>4.2. SAR and QSAR, physico chemical factors and biological activities. Factors governing ability of drugs.</p> <p>4.3. General methods of drug synthesis. Analgesics(phenazones and phenylbutzone as examples). Antipyretic (paracetamol) Antibiotics (pencillins, chloramphanicol).</p>	
<p>Unit 5: Introduction to Industrial Catalysis</p>	<p>8 Hours</p>
<p>5.1. Structure and chemical nature of surfaces. Physisorption and chemisorptions. Energy exchange at surface.</p> <p>5.2. Determination of surface area and pore structure of catalysts - physical adsorption methods, X-ray methods, mercury intrusion method, chemisorptions methods.</p> <p>5.3. Determination of surface acidity-TPD method. Catalyst selectivity, effect of pore size on selectivity.</p> <p>5.4. Homogeneous and heterogeneous catalysts. Preparative methods for heterogeneous catalysts- precipitation and coprecipitaion methods, sol gel method, flame hydrolysis.</p>	

<p>5.5. Preparation of Zeolites and silica supports. Mesoporous materials. Introduction to Phase transfer catalysis, biocatalysis, nanocatalysis and polymer supported catalysis.</p> <p>5.6. Application of heterogeneous catalysts in water gas shift reaction, ammonia synthesis, catalytic cracking, Fisher-Tropsch process, three-way catalysis.</p>	
<p>Unit 6: Renewable Energy Sources</p>	<p>8 Hours</p>
<p>6.1. World's reserve of commercial energy sources and their availability, various forms of energy,</p> <p>6.2. Renewable and conventional energy systems, comparison - coal, oil and natural gas, availability, applications, merits and demerits.</p> <p>6.3. Renewable energy sources - solar energy, nature of solar radiation, components- solar heaters, solar cookers, water desalination.</p> <p>6.4. Photovoltaic generation – basics, merits and demerits of solar energy. i) Solid state junction solar cells: - principle of solar cells, Fabrication of CdS/Cu₂S and CdS/CuInSe₂ solar cells, performance testing, stability and efficiency consideration.</p> <p>6.5. Dye sensitized solar cells (DSSC)-Working principle, Fabrication of DSSCs based on TiO₂ and ZnO, stability and performance of dyes.</p>	
<p>Unit 7: Organic semiconductors and electronics</p>	<p>8 Hours</p>
<p>7.1. General overview of organic semiconductors and electronics - Bonding, Conjugation, Hybridization, Electronic structure. Charge injection and transport in organic semiconductors, optical phenomenon.</p> <p>7.2. Representative materials and their processing</p> <p>7.3. Film deposition techniques, structure-property relationships</p> <p>7.4. Patterning, Printing, Encapsulation</p> <p>7.5. Electro-optical devices theory and fabrication of organic Light emitting diodes, thin film transistors, Solar cells, memory devices and sensors.</p>	

MODE OF TRANSACTION

Module	Mark
Unit 1: Chemistry of Nanomaterials	12
Unit 2: Introduction to computational quantum chemistry	6
Unit 3 Supramolecular Chemistry	7
Unit 4: Medicinal Chemistry	7
Unit 5: Introduction to Industrial Catalysis	7
Unit 6: Renewable Energy Sources	7
Unit 7: Organic semiconductors and electronics	7

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M.Sc. CHEMISTRY (CBCSS PATTERN)
SEMESTER IV

COURSE CODE –MCH4P01 RESEARCH PROJECT				
Credit	Hours/week	Weightage		
		Internal	External	Total
4	3	5	30	35

Course Outcomes

CO No.	Expected Course Outcome	Learning Domain	PSO No
	Upon completion of this course, students will be able to;		
CO1	<i>Propose</i> a problem for the project work.	Create	PSO 2 PSO 3 PSO 11
CO2	<i>Summarize</i> review of literature.	Understand	PSO 2
CO3	<i>Design</i> a methodology for carrying out the project work.	Create	PSO 2 PSO 3
CO4	<i>Develop</i> analytical skills in setting up experimental techniques and operate it to determine the data required.	Create Apply	PSO 4
CO5	<i>Measure</i> and interpret the data to draw conclusion.	Understand	PSO 5 PSO 6
CO6	<i>Make</i> a project report.	Create	PSO 7 PSO 11

Mode of Transaction
<p>Experimentation: This involves learning by doing or hands on experience by applying chemical principles.</p> <p>Observation: Measurement of physical parameters and readings.</p>

Mode of Assessment
<p>Internal Assessment (weightage:10)</p> <ul style="list-style-type: none"> a. Literature survey and data collection – 2 weightage b. Interpretation of data & Preparation of Project report – 2 weightage c. Research attitude – 2 weightage d. Viva Voce – 4 weightage
<p>External Assessment (30 Weightage)</p> <ul style="list-style-type: none"> a. Significance and relevance of the project – 5 weightage b. Project report – 8 weightage c. Presentation – 5 weightage d. Viva Voce – 12 weightage

Examination conducted at the end of IV semester

M.Sc. CHEMISTRY (CBCSS PATTERN)
SEMESTER IV

COURSE CODE –MCH4V01				
VIVA VOCE				
Credit	Hours/week	Weightage		
		Internal	External	Total
2	-	0	30	30

Course Outcomes

CO No.	Expected Course Outcome	Learning Domain	PSO No
	Upon completion of this course, students will be able to;		
CO1	Describe Theoretical principles behind chemical and physical phenomena.	Remember	PSO 1 PSO 2
CO2	Outline Theoretical principles in the laboratory experiments.	Remember	PSO 1 PSO 2
CO3	Judge scientific statements.	Evaluate	PSO 3

Mode of Assessment	Internal Assessment
	<i>No internal evaluation for viva voce examinations</i>
External Assessment (30 Weightage)	
<i>Based on both the Theory and Practical courses during the programme</i>	
<ol style="list-style-type: none"> 1. Physical & Theoretical Chemistry – Theory courses 5 Weightage 2. Physical Chemistry – Practical courses 5 Weightage 3. Inorganic Chemistry – Theory courses 5 Weightage 4. Inorganic Chemistry – Practical courses 5 Weightage 5. Organic Chemistry – Theory courses 5 Weightage 6. Organic Chemistry – Practical courses 5 Weightage 	

Examination conducted at the end of IV semester