

## **Study Scheme & Syllabus**

**For**  
**M.Sc. Chemistry**  
**(First to Fourth Semester)**  
**Program Code-CHEM-401**



**Syllabi Applicable for Admissions in 2016 onwards**

**DEPARTMENT OF CHEMISTRY**  
**RIMT UNIVERSITY, MANDIGOBINDGARH, PUNJAB**

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**SECTION 1****Vision & Mission of the University****VISION**

To become one of the most preferred learning places a center of excellence to promote and nurture future leaders who would facilitate desired change in the society.

**MISSION**

- To impart teaching and learning through cutting-edge technologies supported by the world-class infrastructure.
- To empower and transform young minds into capable leaders and responsible citizens of India instilled with high ethical and moral values.
- To all-round development of students through education and innovation.

**SECTION 2****Vision and Mission of the Department****VISION**

Our vision is to enhance our reputation as a world-class teaching and research institution which is recognized for its innovation, excellence, and discovery and attracts the best students and staff worldwide. Our main objective is to increase the proficient and positive use of knowledge and wisdom and to encourage fraternity among children, people, states, and nations, looking for a true understanding among all, based on respect for the ideology, social belief, faith, race, and gender individual.

**MISSION**

- To provide a high-quality educational experience for undergraduate and graduate students that enables them to become leaders in their chosen professions.
- Department strives towards excellence in all the fields of teaching, research, and public service by developing outstanding research and academic programs and providing high-quality of education to best satisfy the learners.
- We, at the department of chemistry, constantly afford to enrich our syllabus. and programs according to current trends in higher education. All the courses in the program are. carefully designed based on the guideline of NTA and UGC.
- I invite you to explore our department website to cognize the academic and top-notch research of the department.
- To develop the leadership quality in the students in the field of science, innovation specially chemistry and chemistry involved in technology.

**SECTION 3****About the Program**

Chemistry is the science of matter and the changes it undergoes. The science of matter is also addressed by physics, but while physics takes a more general and fundamental approach, chemistry is more specialized, being concerned with the composition, behavior, structure, and properties of matter, as well as the changes it undergoes during chemical reactions.

This Program is an Outcome Based Education model which is a 2-year, 4 Semester Full time Program of 97 credits (CBCS) and Grading Evaluation System.

**SECTION 4****Program Educational Objectives (PEOs), Program Outcomes (POs) and Program Specific Outcomes (PSOs)**

The PEOs are **broad statements** that describe the career and professional accomplishments that the program is preparing its graduates to achieve in two years subsequent to receiving the degree. The PEOs of the ‘**MSc Chemistry**’ program are as follows:

**PROGRAMME EDUCATION OBJECTIVES (PEOs)**

<b>PEO1</b>	<b>Creative Thinking</b>	Students will be able to think creatively (divergently and convergent) to propose novel ideas in explaining facts and figures or providing new solution to the problems in chemistry.
<b>PEO2</b>	<b>Interdisciplinary Approach</b>	Students will realize how developments in any science subject helps in the development of other science subjects and vice-versa and how interdisciplinary approach helps in providing better solutions and new ideas for the sustainable developments.
<b>PEO3</b>	<b>Personality Development</b>	Students will imbibe ethical, moral and social values in personal and social life leading to highly cultured and civilized personality.
<b>PEO4</b>	<b>Skills in research and industrial field</b>	Students will build a scientific temper and will be able to learn the necessary skills to succeed in research or industrial field
<b>PEO5</b>	<b>Communication Skills and Environmental monitoring</b>	Students will develop various communication skills such as reading, listening, speaking, etc., which we will help in expressing ideas and views clearly and effectively.

**PROGRAMME OUTCOMES (POs)**

<b>PO 1</b>	The master's degree program is structured to provide students a thorough grasp of the basics and developments of chemistry, including all concepts and viewpoints.
<b>PO 2</b>	It will aid in the development of problem-solving abilities based on chemical principles, as well as providing students with a wide theoretical and practical grounding in all areas of chemistry, with a focus on qualitative and quantitative techniques.
<b>PO 3</b>	Students will be able to think creatively to come up with new ways to present facts and numbers, as well as innovative solutions to chemical issues. Observational abilities and the ability to make logical conclusions from scientific tests will also be honed.
<b>PO 4</b>	Students will learn how advances in one scientific field assist in the advancement of other science disciplines and vice versa, as well as how an interdisciplinary approach aids in the creation of better solutions and new ideas for long-term sustainability.
<b>PO 5</b>	Students will be able to comprehend environmental challenges including global warming, climate change, acid rain, and ozone depletion, as well as raise societal awareness.
<b>PO 6</b>	Students will develop a scientific mindset and be able to gain the skills needed to excel in research or industry. They will also learn how to use scientific tools, as well as organize and carry out laboratory experiments.
<b>PO 7</b>	Aptitude to acquire newer knowledge and skills, assimilate and adapt them to be ready to confront uncharted environment scientifically and confidently.
<b>PO 8</b>	A strong business sense to explore entrepreneurial opportunities and leverage managerial & leadership skills for initiating, leading & managing start-ups as well as professionalizing and growing businesses.
<b>PO 9</b>	Capability of mapping out a team's or organization's tasks and setting direction, formulating an inspiring vision, forming a team to help achieve the vision, motivating and inspiring team members to engage with that vision, and using management skills to guide people to the right destination in a smooth and efficient manner.
<b>PO 10</b>	Exhibit understanding to assess the impact of managerial decisions and business priorities on the societal, economic and environmental aspects for sustainable development.

**PROGRAMME SPECIFIC OBJECTIVES (PSOS)**

<b>PSO1</b>	Students will understand the basic concepts, fundamental principles, and the scientific theories related to various scientific phenomena and their relevancies in the day-to-day life. They will also be able to acquire knowledge about the fundamentals and applications of chemical and scientific theories
<b>PSO2</b>	Students will find that every branch of science and technology is related to Chemistry. They will develop scientific outlook not only with respect to science subjects but also in all aspects related to life.
<b>PSO3</b>	Students will become familiar with the different branches of chemistry like analytical, organic, inorganic, physical, environmental, polymer and biochemistry.
<b>PSO 04</b>	As a health professional the students shall have an added responsibility towards the society.



**SECTION 5****Curriculum / Scheme with Examination  
Grading Scheme****SEMESTER WISE SUMMARY OF THE PROGRAM: M.Sc CHEMISTRY**

<b>S.No</b>	<b>Semester</b>	<b>No. of contact hours</b>	<b>Marks</b>	<b>Credits</b>
1	1	32	900	25
2	2	28	700	22
3	3	28	500	25
4	4	28	500	25

**Program Name- M.Sc. Chemistry  
EXAMINATION GRADING SCHEME**

<b>Marks percentage range</b>	<b>Grade</b>	<b>Grade point</b>	<b>Qualitative meaning</b>
<b>80-100</b>	O	10	OUTSTANDING
<b>70-79</b>	A+	9	EXCELLENT
<b>60-69</b>	A	8	VERY GOODE
<b>55-59</b>	B+	7	GOOD
<b>50-54</b>	B	6	ABOVE AVERAGE
<b>45-49</b>	C	5	AVERAGE
<b>40-44</b>	P	4	PASS
<b>0-39</b>	F	3	FAIL
<b>AB</b>			ABSENT

**Percentage calculation: CGPA\*10**

**SECTION 6****Detailed Syllabus with Course Outcomes**

First Semester

Subject		Contact Hours/Week			Credit	Evaluation Scheme (% of Total Marks)					Exam Duration (Hours)
Code	Title	L	T	P		CW	LWA	MTE	ETE	Total	
MCHE-1101	Inorganic Chemistry-I(Transition Metal Chemistry)	3			3	16	---	24	60	100	
MCHE-1102	Organic Chemistry –I (Reaction Mechanism-I)	3			3	16	---	24	60	100	
MCHE-1103	Physical Chemistry-I(Thermodynamics)	3			3	16	---	24	60	100	
MCHE-1104	Molecular Spectroscopy-I	4			4	16	---	24	60	100	
MCHE-1105	Supramolecular Chemistry	3			3	16	---	24	60	100	
MCHE-1106	Inorganic Chemistry Lab-I			6	3	---	40	---	60	100	
MCHE-1107	Physical Chemistry Lab I			6	3	----	40	----	60	100	
MCOP-1101	Basic of Computer	2			2	----	60	----	40	100	

## Program Code: MCHE-401

	Programming using C++										
MCOP-1102	Computer Lab			2	1	----	40	-----	60	100	
<b>Total</b>					<b>25</b>						

L—Lecture, T- Tutorial, P-Practical, CWA-Class work Assessment, LWA-Lab work Assessment, MTE- Mid Term Exam, ETE- End Term Exam

### Second Semester

Subject		Contact Hours/Week			Credit	Evaluation Scheme (% of Total Marks)					Exam Duration (Hours)
Code	Title	L	T	P		CWA	LWA	MTE	ETE	Total	
MCHE-1201	Inorganic Chemistry-II (Reaction Mechanism and Organometalics)	3			3	1 6	---	24	60	100	
MCHE-1202	Organic Chemistry-II (Reaction Mechanism-II)	3			3	1 6	---	24	60	100	
MCHE-1203	Physical Chemistry-II (Quantum Chemistry)	3			3	1 6	---	24	60	100	
MCHE-1204	Molecular Spectroscopy-II	4			4	1 6	---	24	60	100	
MCHE-1205	Bioorganic & Medicinal Chemistry	3			3	1 6	---	24	60	100	
MCHE-1206	Organic Chemistry Lab-I			6	3	--	40	---	60	100	

Program Code: MCHE-401

MCHE-1207	Electroanalytical Lab			6	3	--	40	----	60	100	
<b>Total</b>					<b>22</b>						

L-- Lecture

T-- Tutorial

P---Practical

CWA Class work Assessment

LWA Lab work Assessment

MTE Mid Term Exam

ETE End Term Exam

### Third Semester

Subject		Contact Hours/Week			Credit	Evaluation Scheme (% of Total Marks)					Exam Duration (Hours)
Code	Title		T	P		CWA	LWA	MTE	ETE	Total	
MCHE-2301	Inorganic Chemistry-III (Radiochemistry & Nanochemistry)				3	16	--	24	60	100	
MCHE-2302	Organic Chemistry – III(Photochemistry& Pericyclic Reactions)				3	16	--	24	60	100	
MCHE-2303	Macromolecule and Polymer Chemistry				3	16	--	24	60	100	
MCHE-2304	Spectroscopy in structure elucidation and asymmetric synthesis				4	16	--	24	60	100	
MCHE-2305	Biochemistry Lab			6	3						
	Dissertation/Optional Subjects				9	16	--	24	60	100	
MPRO-2405	Dissertation				9	16	--	24	60	100	
MCHE-2306	Coordination Chemistry				3	16	--	24	60	100	
MCHE-2307	Nuclear Chemistry				3	16	--	24	60	100	

Program Code: MCHE-401

MCHE-2308	Inorganic Chemistry Lab--II			6	3						
MCHE-2309	Stereochemistry: Conformation and mechanism				3	16	--	24	60	100	
MCHE-2310	Organic Synthesis-IV				3	16	--	24	60	100	
MCHE-2311	Organic Chemistry Lab-II			6	3						
MCHE-2312	Chemistry of Materials				3	16	--	24	60	100	
MCHE-2313	Physical Chemistry-III				3	16	--	24	60	100	
MCHE-2314	Physical Chemistry lab -II			6	3						
<b>Total</b>					<b>25</b>						

L-- Lecture

T-- Tutorial

P---Practical

CWA Class work Assessment

LWA Lab work Assessment

MTE Mid Term Exam

ETE End Term Exam

### Fourth Semester

Subject		Contact Hours/Week			Credit	Evaluation Scheme (% of Total Marks)					Exam Duration (Hours)
Code	Title	L	T	P		CWA	LWA	MTE	ETE	Total	
MCHE-2401	Bio-Inorganic Chemistry	3			3	16	--	24	60	100	
MCHE-2402	Biosynthesis of Natural Products	3			3	16	--	24	60	100	
MCHE-2403	Bio-Physical Chemistry	3			3	16	--	24	60	100	
MCHE-2404	Analytical Chemistry	4			4	16	--	24	60	100	
MCHE-2405	Physical Chemistry Lab-III			6	3						

Program Code: MCHE-401

	Dissertation/Optional Subjects	9		9	16	--	24	60	100
MPRO-2405	Dissertation			9	16	--	24	60	100
MCHE-2406	Inorganic Chemistry - IV	3		3	16	--	24	60	100
MCHE-2407	Photo Inorganic Chemistry	3		3	16	--	24	60	100
MCHE-2408	Inorganic Chemistry Lab-III		6	3					
MCHE-2409	Modern Synthetic Reactions and Rearrangements	3		3	16	--	24	60	100
MCHE-2410	Heterocyclic Chemistry	3		3	16	--	24	60	100
MCHE-2411	Organic Chemistry Lab-III		6	3					
MCHE-2412	Biofuels	3		3	16	--	24	60	100
MCHE-2413	Surface Chemistry	3		3	16	--	24	60	100
MCHE-2414	Physical Chemistry Lab-IV		6	3					
<b>Total</b>				<b>25</b>					

L-- Lecture

T-- Tutorial

P---Practical

CWA Class work Assessment

LWA Lab work Assessment

MTE Mid Term Exam

ETE End Term Exam



**EVALUATION**

1. There shall be two Mid Term Examination (MTE) of 24% Marks (24 marks) in each semester. Average of two is considered for final internal assessment.
2. There shall be continuous class work assessment (CWA) of 16% (16 Marks) of theory subjects
3. End Term examination (ETE) will be of 60% of total marks (60 marks).
4. Each practical examination shall be of 3 hours duration.
5. There shall be continuous lab work assessment (LWA) for practical of 40% marks (40 marks). The final examination will be of 60% marks (60 marks).

**Pattern of end-semester question paper**

The question paper consist of three sections A, B & C.

1. Section-A is compulsory consisting of 6 short answer type questions (2 marks) from the whole syllabus. Total marks to this section are 12. There will be no choice in this section.
2. Section-B consists of 8 questions. Students will attempt any six questions. Each question carries 4 Marks.
3. Section-C consists of 4 questions. Students will attempt any three questions. Each question carries 8 Marks.



Program Name: Masters in Chemistry

Program Code: MCHE-401

# **SYLLABUS**

## **SEMESTER-I**

**SUBJECT TITLE: Inorganic Chemistry-I (Transition Metal Chemistry)****SUBJECT CODE: MCHE-1101****SEMESTER: I****CONTACT HOURS/WEEK:**

Lecture (L)	Tutorial (T)	Practical (P)	Credit (C)
3	0	0	3

**Internal Assessment: 40****End Term Exam: 60****Duration of Exam: 3 Hrs**

**Course Objective:** To impart advanced knowledge of symmetry and group theory and  $\pi$ -acid ligands, chemistry of transition metals.

### Section-A

#### 1. Symmetry and Group Theory: (10 Hrs)

Symmetry Elements, Symmetry Operations, Symmetry Elements commonly occurring molecules like  $\text{NH}_3$ ,  $\text{CH}_4$ ,  $\text{SF}_6$ ,  $\text{PF}_5$ ,  $\text{SF}_4$ ,  $\text{Ni}(\text{CO})_4$ ,  $\text{Fe}(\text{CO})_5$ , determination of point groups, use of character table for determining the reducible and irreducible representation, determination of symmetry of atomic orbitals under different point groups, determination of atomic orbital involved in  $sp$ ,  $sp^2$ ,  $sp^3$ ,  $dsp^2$ ,  $d^2sp^3$  hybridization on basis of group theory and quantitative discussion on concept of hybridization

### Section-B

#### 2. Complexes of $\pi$ -Acid Ligands: (10 hrs)

Acceptor character of  $\text{CO}$ ,  $\text{N}_2$ ,  $\text{O}_2$ ,  $\text{NO}$  molecules in terms of MOEL diagrams,  $\pi$  acid ligands of other groups of periodic table. Semi-bridging in metal carbonyls and isocyanides of metals. Magnetic, IR and X-ray diffraction evidence of their structure, acidity and softness, Symbiosis and antisymbiosis, complexes of unsaturated organic molecules (bonding with  $\text{C}_2\text{H}_4$  only).

Structures & the IR spectral properties representative transition metal carbonyl complexes.

### Section-C

#### 3. Chemistry of Transition Metals-I: (13 Hrs.)

Program Code: MCHE-401

LS coupling, derivation of spectroscopic terms for  $d^1$  to  $d^9$  electronic configurations, correlation diagram for  $d^2$  ion in octahedral field, splitting of  $d^1$  to  $d^9$  terms in an octahedral and tetrahedral field.

Selection rules of d-d transitions. Vibronic and spin orbit coupling, effecting of weak to strong cubic fields on R-S terms, Comparison of CFSE values of  $d^1$  to  $d^9$  ions in terms of orbit splitting and R-S term splitting. Effect of CFSE on thermodynamic properties, lattice energy, heat of hydration heat of ligation and spinal structure. Orgel and Tanabe Sugano diagrams, spectra of octahedral, tetrahedral, distorted octahedral (Jahn Teller Effect) and square planer complexes spectrochemical series, nephelauxetic effect, Calculation of  $\Delta_o$  and  $10 Dq$  from spectral data. Molecular orbital theory-composition of ligand groups, orbitals, sigma and pi-molecular orbitals MOEL, diagrams of  $O_h$ ,  $T_d$  and  $D_{4h}$  complexes with and without pi-bonds, charge transfer spectra.

**4. Chemistry of Transition Metals –II: (12 hrs)**

Magnetic properties of transition metal ions and free ions presentive, Diamagnets and Perromgnetier & ferrongrets. Effects of L-S coupling on magnetic properties. Temperature independent paramagnetism (TIP) in terms of crystal field theory (CFT) and molecular orbital theory (MOT). Quenching of orbital anglor momentum by crystal fields in complexes in terms of term-splitting. Effect of spi-orbit coupling and A, E & T states, Mixing in effect, first order and second order zeeman effects. Spinpaired and spin-free equilibria in complexes magnetic properties of polynuclear complexes, involving OH,  $NH_2$  and CN bridges.

**Course Outcomes:**

CO1	MCHE-1101.1	Learning the basic principles of coordination chemistry
CO2	MCHE-1101.2	Learning the symmetry operation using group theory
CO3	MCHE-1101.3	Understand the coordination chemistry of pi acid complexes
CO4	MCHE-1101.4	Understand the concept of coordination chemistry in daily life

**Books Recommended:**

1. R.S. Drago, Physical Methods in Inorganic Chemistry Ist and 2nd Edition.
2. F.A. Cotton, Chemical Application of group theory, 2nd Edition.

**Program Code: MCHE-401**

3. B.N. Figgis, Introduction to Ligand Fields, First Edition.
4. F.A.Cotton & G. Wilkinson, Advanced Inorganic Chemistry, 5th Edition.
5. F.Basolo and R.C. Johnson, Coordination Chemistry, 1st Edition.
6. J.E. Hukey, Inorganic Chemistry, 3rd Edition.
7. A.B.P. Lever, Inorganic Electronic-Spectroscopy, 2nd Edition.
8. A. Earnshaw, Introduction to Magnetic Chemistry, 1st Edition

Program Code: MCHE-401

**SUBJECT TITLE: Organic Chemistry–I (Reaction Mechanism-I)****SUBJECT CODE: MCHE-1102****SEMESTER: I****CONTACT HOURS/WEEK:**

Lecture (L)	Tutorial (T)	Practical (P)	Credit (C)
3	0	0	3

**Internal Assessment: 40****End Term Exam: 60****Duration of Exam: 3 Hrs**

**Course Objective:** To introduce reaction mechanism of nucleophilic and electrophilic substitutions and free radical reactions

### Section-A

#### 1. Reaction Mechanism: Structure and Reactivity: (10 Hrs)

Type of mechanisms, types of reactions, thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond's postulate, Curtin-Hammett principle. Potential energy diagrams, transition states and intermediates, methods of determining mechanisms, isotope effects. Hard and soft acids and bases. Generation, structure, stability and reactivity of carbocations, carbanions, free radicals, carbenes and nitrenes. Effect of structure on reactivity- resonance and field effects, steric effect, quantitative treatment. The Hammett equation and linear free energy relationship, substituent and reaction constants. Taft equation.

#### 2. Aliphatic Nucleophilic Substitutions: (10 Hrs)

The SN<sub>2</sub>, SN<sub>1</sub>, missed SN<sub>1</sub> and SN<sub>2</sub> and SET mechanisms. The neighbouring group mechanism, neighbouring group participation by  $\pi$  and  $\sigma$  bonds, anchimeric assistance. Classical and nonclassical carbocations, phenonium ions, norbornyl system, common carbocation rearrangements. Application of NMR spectroscopy in the detection of carbocations. The SN<sub>i</sub> mechanism, Nucleophilic substitution at an allylic, aliphatic trigonal and a vinylic carbon. Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction

medium, phase transfer catalysis and ultrasound, ambident nucleophile, regioselectivity. Gabriel synthesis

### Section-B

#### 3. Aromatic Nucleophilic Substitution: (5 Hrs)

The S<sub>N</sub>Ar, S<sub>N</sub>1, benzyne and S<sub>RN</sub>1 mechanisms, Reactivity – effect of substrate structure, leaving group and attacking nucleophile. The von Richter, Sommelet-Hauser, and Smiles rearrangement

#### 4. Aliphatic Electrophilic Substitutions: (5 Hrs)

Bimolecular mechanisms- S<sub>E</sub>2 and S<sub>E</sub>i. The S<sub>E</sub>1 mechanism, electrophilic substitution accompanied by double bond shifts. Effect of substrates, leaving group and the solvent polarity on the reactivity, Hell-Volard-Zelinsky reaction,

### Section-C

#### 5. Aromatic electrophilic substitution: (5 Hrs)

The arenium ion mechanism, orientation and reactivity in mono substitution and disubstituted aromatics, energy profile diagram, the ortho/para ratio, ipso attack, orientation in other ring systems, quantitative treatment of reactivity in substrates and electrophiles. Diazo coupling, Vilsmeier reaction, Gatterman-Koch reaction, Bechmann reaction, Hoesch reaction.

#### 6. Free Radical Reactions: (5 Hrs)

Types of free radical reactions, free radical substitution mechanism, mechanism at an aromatic substrate, neighbouring group assistance. Reactivity for aliphatic and aromatic substrates at a bridgehead. Reactivity in the attacking radicals. The effect of solvents on reactivity. Allylic halogenation (NBS), oxidation of aldehydes to carboxylic acids, autooxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts. Sandmeyer reaction. Free radical rearrangement. Hunsdiecker reaction

#### Course Outcomes:

CO1	MCHE-1102.1	Basic Principles of the organic reaction mechanism
CO2	MCHE-1102.2	Mechanism and stereochemistry of S <sub>N</sub> <sup>1</sup> and S <sub>N</sub> <sup>2</sup> reactions and neighboring group participation in substitution reactions

## Program Code: MCHE-401

CO3	MCHE-1102.3	Aromatic nucleophilic and electrophilic Substitution reactions with mechanism
CO4	MCHE-1102.4	Mechanism and stereochemistry of Elimination reactions

**Books Recommended:**

1. Organic Reaction Mechanism by Jerry March 5<sup>th</sup> Edition
2. Advanced Organic Chemistry by Francis Carey, Vol. A and Vol. B



**SUBJECT TITLE: Physical Chemistry –I (Thermodynamics)****SUBJECT CODE: MCHE-1103****SEMESTER: I****CONTACT HOURS/WEEK:**

Lecture (L)	Tutorial (T)	Practical (P)	Credit (C)
3	0	0	3

**Internal Assessment: 40****End Term Exam: 60****Duration of Exam: 3 Hrs**

**Course Objective:** To impart advanced knowledge of thermodynamics and chemical dynamics

#### **Section-A**

##### **1. Thermodynamics I: (10 Hrs)**

Laws of Thermodynamics, free energy, chemical potential and entropy, Determination of partial molar free energy, volume and heat content, and their significances. Concept of fugacity and determination of fugacity in liquids and gases. Non ideal systems: Excess functions for non-ideal solutions, Activity, activity Coefficient. Debye Huckel theory for activity coefficient of electrolytic solutions; determination of activity and activity coefficient, ionic strength. The Debye Huckel Theory and its applications. Numerical Problems.

#### **Section-B**

##### **2. Non Equilibrium Thermodynamics: (11hrs)**

Thermodynamic criteria for non equilibrium states, entropy production and entropy flow, entropy balance equations for different irreversible processes (for example heat flow, chemical reaction, etc.), generalized forces and fluxes, non equilibrium stationary states, phenomenological equations, microscopic reversibility and Onsager's reciprocity relations, electrokinetic phenomena, diffusion, electric conduction, irreversible thermodynamics for biological systems, coupled reactions.

#### **Section-C**

##### **3. Statistical Thermodynamics: (12 Hrs.)**

## Program Code: MCHE-401

Thermodynamics probability and most probable distribution of a system, Maxwell-Boltzmann distribution law. Ensembles: canonical, grand canonical and micro canonical. Partition functions; translational, rotational, vibrational and electronic. Calculation of thermodynamic properties in terms of partition functions. Application of partition function to calculate heat capacities and equilibrium constants, relation between entropy and thermodynamic probability, Fermi-Dirac and Bose-Einstein statistics. Numerical problems.

**4. Chemical Dynamics: (12Hrs)**

Methods of determining rate laws, collision theory of reaction rates, steric factor, activated complex theory, Arrhenius equation, concept of energy of activation, potential energy surfaces; ionic reactions, kinetic salt effects, steady state kinetics, kinetic and thermodynamic control of reactions. Lindemann-Christiansen hypothesis, Hinshelwood treatment and Rice Ramsperger-Kassel-Marcus (RRKM) theories of unimolecular reactions. General features of fast reactions, study of fast reactions by flow method, relaxation method, flash photolysis and nuclear magnetic resonance method. Dynamic chain (hydrogen-bromine reaction, pyrolysis of acetaldehyde, decomposition of ethane), photochemical (hydrogen bromine and hydrogen-chlorine reactions)

**Course Outcomes:**

CO1	MCHE-1103.1	Understand of the laws of thermodynamics and their applications with Study fugacity and activity coefficient and its determination
CO2	MCHE-1103.2	Understand the Thermodynamic criteria for non-equilibrium states, Onsager's reciprocity relations, electrokinetic phenomena, and thermodynamics for biological system.
CO3	MCHE-1103.3	Analyze the most probable distributions of a system among the energy levels using principles of statistical thermodynamics.
CO4	MCHE-1103.4	Understand the Methods of determining rate laws, collision theory of reaction rates, theories of unimolecular reactions, fast reactions and their study.

**Books Recommended:**

1. Physical Chemistry P.W. Atkins 11th Edition.
2. Thermodynamics for Chemists by S. Glasstone. 7<sup>th</sup> Edition.
3. Chemical kinetics K.J. Laidler 4<sup>th</sup> Edition.
4. Principles of Physical Chemistry, S.H. Maron & C.F. Prutton 2<sup>nd</sup> Edition.
5. Introduction to the Thermodynamics of Biological Processes by D. Jou & J. E. LLebot. 1st Edition.

Program Code: MCHE-401

**SUBJECT TITLE: Molecular Spectroscopy – I****SUBJECT CODE: MCHE-1104****SEMESTER: I****CONTACT HOURS/WEEK:**

Lecture (L)	Tutorial (T)	Practical (P)	Credit (C)
4	0	0	4

**Internal Assessment: 40****End Term Exam: 60****Duration of Exam: 3 Hrs**

**Course Objective:** To acquire knowledge of UV and Visible, NMR, IR, Mass spectroscopy and their applications.

### Section-A

#### 1. General Features of Spectroscopy: (5 Hrs.)

Units and conversion factors. Introduction to spectroscopy, Nature of radiation. Energies corresponding to various kinds of radiation, Experimental techniques, intensities of spectral lines, Selection rules and transition moments, Line widths, Broadening.

#### 2. UV and Visible Spectroscopy of organic molecules: (10 Hrs.)

Measurement techniques, Beer – Lambert's Law, molar extinction coefficient, oscillator strength and intensity of the electronic transition, Frank Condon Principle, Ground and first excited electronic states of diatomic molecules, relationship of potential energy curves to electronic spectra, Chromophores, auxochromes, blue shift, red shift, hypo and hyperchromic effect,  $\sigma$ - $\sigma^*$ ,  $\pi$ - $\pi^*$ ,  $n$ - $\pi^*$  transitions in organic molecules, Woodward rules for conjugated dienes and  $\alpha$ ,  $\beta$ -unsaturated carbonyl groups, extended conjugation and aromatic sterically hindered systems, Quantitative applications.

### Section-B

#### 3. Nuclear Magnetic Resonance Spectroscopy: (10 Hrs.)

PMR: Natural abundance of  $^{13}\text{C}$ ,  $^{19}\text{F}$  and  $^{31}\text{P}$  nuclei; The spinning nucleus, effect of external magnetic field, precessional motion and frequency, Energy transitions, Chemical shift and its measurements. Factors influencing chemical shift, anisotropic effect; Integrals of protons, proton exchange, spin-spin coupling- splitting theory, one, two and three bond coupling, virtual, long

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range and allylic coupling, magnitude of coupling constant; factors affecting the coupling constant, Chemical and magnetic equivalence, First and second order spectra, A<sub>2</sub>, AB, AX, AB<sub>2</sub>, AX<sub>2</sub>, A<sub>2</sub>B<sub>2</sub> and A<sub>2</sub>X<sub>2</sub> spin systems, Simplification of complex spectra (solvent effect, field effect, double resonance and lanthanide shift reagents), CW and FT NMR, Relaxation processes, T<sub>1</sub> and T<sub>2</sub> measurements, Applications of PMR in structural elucidation of simple and complex compounds.

<sup>13</sup>C-NMR: Resolution and multiplicity of <sup>13</sup>C NMR, <sup>1</sup>H-decoupling, noise decoupling, broad band decoupling; Deuterium, fluorine and phosphorus coupling; NOE and origin of nuclear overhauser effect. off-resonance, proton decoupling, Structural applications of 13C-NMR., pulse sequences, pulse widths, spins and magnetization vectors, DEPT, INEPT, Introduction to 2D-NMR, COSY, NOESY, NOE, NOE difference, HSQC spectra

**Section-C**

**4. Infrared Spectroscopy: (5Hrs)**

Frequencies, Factors influencing Vibrational Frequencies (Vibrational Coupling, Hydrogen Bonding, Electronic effect, Bond Angles, Field Effect). Sampling Techniques, Absorption of Common functional Groups, Interpretation, Finger print Regions.

**5. Mass Spectra: (10 Hrs.)**

Introduction, methods of ionization EI & CI, Brief description of LD, FAB, SIMS, FD etc., Ion analysis methods (in brief), isotope abundance, Metastable ions, general rules predicting the fragmentation patterns. Nitrogen rule, determination of molecular ion peak, index of H deficiency, fragmentation patterns for aliphatic compounds, amines, aldehydes, Ketones, esters, amides, nitriles, carboxylic acids ethers, aromatic compounds etc.

**Course Outcomes:**

CO1	MCHE-1104.1	Basic concept involved in molecular spectroscopy.
CO2	MCHE-1104.2	Explain the behaviour of molecular systems in external electromagnetic field.
CO3	MCHE-1104.3	Understand the principles and theories of rotational, vibrational, UV-Vis, Fluorescence, Mass and NMR spectroscopy methods.
CO4	MCHE-1104.4	Interpret the molecular spectra and find molecular properties from molecular spectra.

**Books Recommended:**

1. Pavia, Lampman & Kriz, Introduction to Spectroscopy 5th Edition
2. C.N Banwell "Fundamentals of Molecular Spectroscopy" 4<sup>th</sup> Edition
3. R. M. Silverstein, G.C. Bassler, T.C. Morrill, "Spectrometric Identification of Organic Compounds." 3<sup>rd</sup> Edition
4. W. Kemp, "Organic Spectroscopy" 3<sup>rd</sup> Edition.
5. D.H. Williams, I. Fleming, "Spectroscopic Methods in Organic Chemistry" 6<sup>th</sup> Edition.
6. R.C. Banks, E.R. Matjeka, G. Mercer, "Introductory Problems in Spectroscopy" 1<sup>st</sup> Edition

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**SUBJECT TITLE: Supramolecular Chemistry****SUBJECT CODE: MCHE-1105****SEMESTER: I****CONTACT HOURS/WEEK:**

Lecture (L)	Tutorial (T)	Practical (P)	Credit (C)
3	0	0	3

**Internal Assessment: 40****End Term Exam: 60****Duration of Exam: 3 Hrs**

**Course Objective:** To impart advanced knowledge of supramolecular chemistry and their applications

### Section-A

#### 1. Concepts: (5hrs)

Definition and Development of Supramolecular Chemistry, classification of Supramolecular Host-Guest compounds, Pre- organization and Complementarily, Receptors, Nature of Supramolecular interactions.

#### 2. Cation Binding Host: (10hrs)

Crown ethers, Lariat ether and Podands, Cryptands, spherands, selectivity, Macro cyclic, Macrobicyclic and Template effects, soft ligands, calixarenes, carbon donor and  $\pi$ - acid ligands, siderophores.

### Section-B

#### 3. Binding of anions: (10hrs)

Biological anion receptors, concepts on anion host design, From cation to anion hosts- a simple change in pH, Guanidinium- based receptors, Neutral receptors, organometallic receptors, coordination interactions.

#### 4. Binding of Neutral Molecules: (6hrs)

Inorganic solid state clathrate compounds, solid state clathrates of organic hosts, intracavity complexes of neutral molecules, supramolecular chemistry of fullerenes.

**Section-C****5. Crystal Engineering: (7hrs)**

Concepts, crystal structure prediction, Crystal Engineering with hydrogen bonds, weak hydrogen bonds, hydrogen bonds to metals and metal hydrides,  $\pi$ -  $\pi$  stacking, coordination polymers.

**6. Molecular Devices: (7hrs)**

Introduction, Supramolecular photochemistry, molecular electronic devices: Switches, wires and rectifiers, machines based on catenanes and rotaxanes.

**Course Outcomes:**

CO1	MCHE-1105.1	Understand the basics of supramolecular chemistry
CO2	MCHE-1105.2	Understand the reactivity, analysis, and significance of crystal engineering
CO3	MCHE-1105.3	Understand the mechanism and binding of host cation and anions molecules
CO4	MCHE-1105.4	Understand the basics of electronic devices

**Book Recommended:**

1. J.W Steed and J.L Atwood, Supramolecular chemistry, John Wiley & Sons, Ltd. New York. 2<sup>nd</sup> Edition

Program Code: MCHE-401

**SUBJECT TITLE: Inorganic Chemistry Lab-I**

**SUBJECT CODE: MCHE-1106**

**SEMESTER: I**

**CONTACT HOURS/WEEK:**

Lecture (L)	Tutorial (T)	Practical (P)	Credit (C)
0	0	6	3

**Internal Assessment: 40**

**End Term Exam: 60**

**Duration of Exam: 3 Hrs**

**Course Objective:** To teach the synthesis of inorganic complexes and their characterization with Instrumental techniques

### PREPARATION AND ESTIMATIONS

1. Preparation of Tris-thiourea cuprous chloride
2. Estimation of Cu, and Chloride.
3. Preparation of Hexamine-cobalt (III) chloride.
4. Estimation of cobalt.
5. Preparation of Tin tetraiodide.
6. Estimation of Sn.
7. Preparation of  $K_3[Fe(C_2O_4)_3]$ .
8. Estimation of iron
9. Preparation of Hg  $[Co(NCS)_4]$
10. Simultaneous estimation of Hg and Co.
11. Preparation of  $(NH_3)_2HgCl_2$ .
12. Estimation of Hg.
13. Mercuration of phenol and separation of the compound into o—, and p—, isomers.
14. Preparation of  $K_3[Cr(C_2O_4)_3]$
15. Estimation of Cr and oxalate.
16. Spectrophotometric Estimation of
  - (a) Iron with 1, 10 phenanthroline.
  - (b) Chromium with diphenyl carbazide.
17. Chromatographic separation of ions.
  - (a) Paper chromatography. (b) Thin layer chromatography. (c) Column chromatography

### Course Outcomes:

CO1	MCHE-1106.1	To teach the synthesis of inorganic complexes and their characterization
CO2	MCHE-1106.2	Estimate gravimetrically mixture of three metal ions



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CO3	MCHE-1106.3	Estimate calcium and magnesium by chromatographic
CO4	MCHE-1106.4	Prepare and characterize some metal complexes

**Books Recommended:**

1. Vogel's book on Inorganic Qualitative Analysis 6<sup>th</sup> Edition
2. Vogel's book on Inorganic Quantitative Analysis 6th Edition

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**SUBJECT TITLE: Physical Chemistry Lab – I****SUBJECT CODE: MCHE-1107****SEMESTER: I****CONTACT HOURS/WEEK:**

Lecture (L)	Tutorial (T)	Practical (P)	Credit (C)
0	0	6	3

**Internal Assessment: 40****End Term Exam: 60****Duration of Exam: 3 Hrs**

**Course Objective:** To impart advance knowledge on different analytical techniques for chemical analysis

1. To determine the freezing point depression constant of camphor using naphthalene as solute. Hence determine the molecular weight of acetanilide by Rast's micro method.
2. Determination of molecular weight of a non-volatile substance by measuring elevation of boiling point .
3. Determination of heat of solution of a substance by solubility method
4. To determine the relative strength of acids by study kinetics of hydrolysis of an ester.
5. To determine the iodine value of given sample of oil (Linseed oil),
6. To determine the saponification value of given sample of oil (Ground nut oil),
7. To determine the coefficient of viscosity of given liquid by Ostwald's viscometer.
8. To find the molecular weight of polymer by viscosity measurements,.
9. Determination of surface tension of given liquid by drop no. method by stalgmometer,
10. To determine the C.M.C. of a soap
11. To determine the distribution coefficient of  $I_2$  between  $CCl_4$  and  $H_2O$ ,
12. Determination of specific and molar refraction of a liquid by Abbe refractometer.
13. Determine the refraction equivalents of C, H, and Cl atoms. (J.B. Yadav, page – 165).
14. Study and verify the freundlich adsorption isotherm for adsorption of  $CH_3COOH$  from its aqueous solution by activated charcoal. (Findlay, page 373).

**Course Outcomes:**

CO1	MCHE-1107.1	To impart advance knowledge on different analytical techniques of physical chemistry
CO2	MCHE-1107.2	Determine rate constant of acid Hydrolysis of ester
CO3	MCHE-1107.3	Determine relative strength of strong acids by studying the kinetics of hydrolysis of ester
CO4	MCHE-1107.4	To impart advance knowledge on different analytical techniques of physical chemistry

**Books Recommended:**

1. Findlay's Practical Physical Chemistry 9th Edition
2. Advanced Practical Physical Chemistry by J.B. Yadav 16<sup>th</sup> Edition

**Basics of Programming using C<sup>++</sup>**

**To be prepared by concerned department**

**Computer Lab**

**To be prepared by concerned department**



Program Name: Masters in Chemistry

Program Code: MCHE-401

## **SEMESTER-II**

Program Code: MCHE-401

**SUBJECT TITLE: Inorganic Chemistry-II (Reaction Mechanism and Organometallics)****SUBJECT CODE: MCHE-1201****SEMESTER: II****CONTACT HOURS/WEEK:**

Lecture (L)	Tutorial (T)	Practical (P)	Credit (C)
3	0	0	3

**Internal Assessment: 40****End Term Exam: 60****Duration of Exam: 3 Hrs**

**Course Objective:** To impart advance knowledge of reaction mechanism and organometallics

**Section A****1. Reaction Mechanisms of Transition Metal Complexes: (15Hrs.)**

Introduction, ligand replacement reactions, classification of mechanisms, Water exchange rates, formation of complexes from aqueous ions, anation, reaction, aquation and base hydrolysis attack on ligands, reactions, of square planar complexes, mechanism of ligand displacement reactions; metal carbonyl reactions, reactions of binuclear carbonyls, associative reactions, species with 17 electron, electron transfer processes outer and inner sphere. The Marcus theory, doubly bridged inner-sphere transfer, other electron transfer reactions; two electron transfers, Non-complementary reaction, Ligand exchange via electron exchange, reductions by hydrated electrons, stereochemical non-rigidity, stereochemically non-rigid coordination compounds, Trigonal bipyramidal molecules, systems with coordination number six or more, isomerization and recombinations, tris chelate complexes, metal carbonyl scrambling cluster, rotation within Co shells.

**Section B****2. Reaction at Coordinated Ligands: (5 Hrs.)**

Hydrolysis of amino acid esters and peptides and amides, Aldol condensation; Imine formation, hydrolysis and substituent exchange. Template effect and macrocyclic ligands

**Section C****3. Organometallics: (25Hrs.)**

I. The basis of 18e- Rule, Exceptions to eighteen electron rule.

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- II. Preparation of olefin Transition Metal Complexes.
- III. Molecular orbital, Description of bonding of two electron ligands to Transition Metals.
- IV. Preparation of  $\pi$ - enyl complexes, Molecular orbital description of ligands to transition metals.
- V. Dynamic equilibria in allyl complexes.
- VI. Differences between unconjugated & conjugated olefin ligands.
- VII. The bonding of cyclobutadiene to Transition metals.
- VIII. Preparation of cyclobutadiene complexes.
- IX. Classification, Nomenclature of cyclopentadienyl complexes, Preparation of cyclopentadienyl T. M. Complexes.
- X. Molecular orbital picture of bonding in ferrocene.
- XI. Organic Chemistry of cyclopentadienyl Transition Metal Complexes.
- XII. Preparation of bis arene complexes, Bonding of Bis-arene complexes.
- XIII. Preparation of cyclopentadienyl complexes.
- XIV. Organometallic Reagents in Organic synthesis.
- XV. Catalysis involving metal complexes intermediates.

**Course Outcomes:**

CO1	MCHE-1201.1	To impart advance knowledge of reaction mechanism and organometallics
CO2	MCHE-1201.2	To impart knowledge about Hydrolysis of amino acid esters and peptides and amides
CO3	MCHE-1201.3	To understand Molecular orbital, Description of bonding of two electron ligands to Transition Metals.
CO4	MCHE-1201.4	Organometallic Reagents in Organic synthesis

**Books Recommended:**

1. F.A. Cotton & G. Wilkinson, Advanced Inorganic Chemistry, 5th Edition.
2. William W. Porterfield, Inorganic Chemistry, 1st Edition.
3. J.E. Huheey, Inorganic Chemistry, 3rd Edition.
4. Principles of Organometallic Chemistry by M.L.H Green, Coward, G.E Coates and K.Wade  
3<sup>rd</sup> Edition

**SUBJECT TITLE: Organic Chemistry–II (Reaction Mechanism-II)****SUBJECT CODE: MCHE-1202****SEMESTER: II****CONTACT HOURS/WEEK:**

Lecture (L)	Tutorial (T)	Practical (P)	Credit (C)
3	0	0	3

**Internal Assessment: 40****End Term Exam: 60****Duration of Exam: 3 Hrs**

**Course Objective:** To impart advanced knowledge of reaction mechanism, addition, elimination and rearrangement reactions

### Section A

#### 1. Addition to Carbon-carbon and Carbon-Heteroatom Multiple Bonds: (15 Hrs)

Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, regio- and chemoselectivity, orientation and reactivity. Addition to cyclopropane ring. Hydrogenation of double and triple bonds, hydrogenation of aromatic rings. Hydroboration. Michael reaction. Sharpless asymmetric epoxidation. Addition of Grignard reagents, organozinc, organolithium and Gilman reagents to carbonyl and unsaturated carbonyl compounds. Use of other organometallic reagents in addition reactions. Wittig reaction, Mechanism of condensation reactions involving enolates – Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin and Stobbe reactions. Hydrolysis of esters and amides, ammonolysis of esters.

### Section B

#### 2. Elimination Reactions: (5 Hrs)

The E2, E1 and E1cB mechanisms and their spectrum. Orientation of the double bond. Reactivity – effects of substrate structures, attacking base, the leaving group and the medium. Mechanism and orientation in pyrolytic elimination.

#### 3. Oxidation Reactions: (7 Hrs)

Introduction. Different oxidative processes. Hydrocarbons- alkenes, aromatic rings, saturated C-H groups (activated and unactivated). Alcohols, diols, aldehydes, ketones, ketals and

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carboxylic acids. Amines, hydrazines, and sulphides. Oxidations with ruthenium tetroxide, iodobenzene diacetate and thallium (III) nitrate, DDQ, PCC, CAN, selenium dioxide, peroxyacids, DCC. Oxidation reactions with special emphasis on Baeyer-viliger reaction, Cannizzaro oxidation-reduction reaction,

**Section C****4. Reduction Reactions: (10 Hrs)**

Introduction. Different reductive processes, Hydrocarbons- alkanes, alkenes, alkynes and aromatic rings, Carbonyl compounds – aldehydes, ketones, acids, ester and nitriles. Epoxides, Nitro, nitroso, azo and oxime groups, Hydrogenolysis. Sodium borohydride, sodium cyano borohydride, LAH, disobutyl aluminium hydride, tin hydride, trialkyl tin hydride, trialkyl silanes, alkoxy substituted LAH, DIBAL, diborane, diisoamyl borane, hexyl borane, 9-BBN, isopinocampheyl and diisopinocampheyl borane. Reduction reactions with particular emphasis on Wolf-Kishner reduction, Clemensen reduction.

**5. Rearrangements: (8 Hrs)**

General mechanistic consideration – nature of migration, migratory aptitude, memory effects. A detailed study of the following rearrangements, Pinacol-pinacolone, Wagner- Meerwein, Demjanov, Benzil-Benzilic acid, Favorskii, Arndt-Eistert synthesis, Neber, Beckmann, Hofman, Curtius, Schmidt, Shapiro reaction, Fries rearrangement

**Course Outcomes:**

CO1	MCHE-1202.1	Basic Principles of organic reaction mechanism
CO2	MCHE-1202.2	Mechanism and stereochemistry of $SN^1$ and $SN^2$ reactions and neighbouring group participation in substitution reactions
CO3	MCHE-1202.3	Aromatic nucleophilic and electrophilic Substitution reactions with mechanism
CO4	MCHE-1202.4	Mechanism and stereochemistry of Elimination reactions

**Books Recommended:**

1. Organic Reaction Mechanism by Jerry March, 5<sup>th</sup> Edition
2. Advanced Organic Chemistry by Francis Carey, Vol A and Vol B



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**SUBJECT TITLE: Physical Chemistry – II ( Quantum Chemistry)****SUBJECT CODE: MCHE-1203****SEMESTER: II****CONTACT HOURS/WEEK:**

Lecture (L)	Tutorial (T)	Practical (P)	Credit (C)
3	0	0	3

**Internal Assessment: 40****End Term Exam: 60****Duration of Exam: 3 Hrs**

**Course Objective:** To impart advance knowledge of basics of quantum chemistry and its applications

### Section A

#### 1. Mathematical Preparation: (10 Hrs)

Matrices, square, diagonal unit, scalar, symmetric, hermitian matrices, operations on matrices, determinants, adjoint and inverse of matrix. Use of Cayley Hamilton theorem to find inverse of a matrix, even and odd functions, well behaved functions. Operators and observables, normality and orthogonality of functions, Hermitian operators. Introduction to differentiation and Integration.

#### 2. Quantum Theory: Introduction and principles and applications: (17 Hrs)

Black Body radiation, planck's radiation law, photoelectric effect, Compton effect, De-Broglie hypothesis, the Heisenberg's uncertainty principle, Rydberg's relation for explaining atomic spectrum of hydrogen. Bohr theory and its limitations. Solution of classical wave equation by separation of variable method, eigen value equation, Hamiltonian operator. Interpretation of  $\Psi$ , Solution of particle in one, two and three dimensional box, degeneracy. Postulates of quantum mechanics, the linear harmonic oscillator, and the rigid rotator, quantization of vibrational and rotational energies.

### Section B

#### 3. Angular Momentum: (6 Hrs)

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Commutative laws, need of polar coordinates, transformation of cartesian coordinates into polar coordinates. Angular momentum of one particle system, orbital angular momentum, the ladder operator method for angular momentum.

**4. The Hydrogen Atom: (4 Hrs)**

Outline of various steps in the solution of the electronic Schrödinger equation for hydrogen atom, Radial and angular parts of the hydrogenic wave functions (atomic orbitals) and their variations for 1s, 2s, 2p, 3s, 3p and 3d orbitals. Significance of Quantum numbers, orbital angular momentum and quantum numbers  $m_l$  and  $m_s$ .

**Section C****5. The Approximation Methods: (5 Hrs.)**

Need for approximation methods, Perturbation and Variation methods and their application to Helium atom.

**6. Chemical Bonding: (3 Hrs)**

Chemical bonding, linear combination of atomic orbitals, overlap integral, coulomb integral, molecular orbital treatment of  $H_2^+$ , Bonding and antibonding orbital of  $H_2^+$

**Course Outcomes:**

CO1	MCHE-1203.1	The subject offers the readers a fundamental understanding of Mathematical tools used in quantum
CO2	MCHE-1203.2	To provide students with a basic understanding of essentials of principle of quantum mechanics
CO3	MCHE-1203.3	Basic understanding of theories of quantum
CO4	MCHE-1203.4	To understand the recent advancement of Chemical bonding, linear combination of atomic orbitals

**Books Recommended:**

1. Quantum Chemistry, Ira N. Levine.
2. Quantum Chemistry, H. Eyring J. Walter and G. E. Kimball. Molecular

**SUBJECT TITLE: Molecular Spectroscopy – II****SUBJECT CODE: MCHE-1204****SEMESTER: II****CONTACT HOURS/WEEK:**

Lecture (L)	Tutorial (T)	Practical (P)	Credit (C)
4	0	0	4

**Internal Assessment: 40****End Term Exam: 60****Duration of Exam: 3 Hrs**

**Course Objective:** To acquire knowledge of rotational vibrational, NQR, Massbauer, Xray diffraction and photoelectron spectroscopy and their applications

### Section A

#### 1. Pure Rotational Spectra: (8 Hrs.)

Classification of molecules according to their moment of inertia. Rotational spectra of diatomic molecules (rigid rotator), Intensities of spectral lines, isotopic substitution effects, non-rigid rotator, polyatomic linear and symmetric top molecules, Stark effect.

#### 2. Vibrational Spectroscopy: (15 hrs)

**Theory of Infrared Absorption:** Harmonic and anharmonic oscillators, absorptions of radiation by molecular vibrations, selection rules, force constant, frequency of vibrational transitions of HCl, vibrations in a polyatomic molecule,  $3N-6$  and  $3N-5$  rules, types of vibrations, overtones, combination and difference bands, examples of CO<sub>2</sub>, SO<sub>2</sub> and H<sub>2</sub>O, Fermi resonance, group vibrations.

**Raman Spectroscopy:** Introduction, selection rules, anisotropic polarizability, Stokes, anti-Stokes lines, vibrational Raman spectra of CO<sub>2</sub> and H<sub>2</sub>O, polarised and depolarised Raman Lines, rule of mutual exclusion.

**Determination of IR/Raman Active Modes:** Significance of nomenclature: used to describe various vibrations, use of symmetry considerations to determining the number of active infrared and Raman Lines (C<sub>2v</sub> molecules).

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**Applications:** Physical state of a sample, cells used, Application of IR in structure elucidation of organic compounds-carbonyls and effect of substituents on it, C-H, N-H, O-H vibrations and H-bonding- unsaturated, mono- and disubstituted aromatic compounds, metal-ligand vibrations, group frequencies of complex ligands-CN stretching and effect of coordination on it, nitro and nitrite and C=O ligands and effect of their coordination with metal ions.

**Section B****3. Nuclear Quadruple Resonance Spectroscopy: (5 Hrs.)**

Introduction, experimental considerations, fundamentals of NOR spectroscopy, origin of EFG, measurement of energy differences between two nuclear spin states, the asymmetry parameter, effects of the magnetic field, interpretation of the spectra, application of the technique to halogen compounds, group elements, transition metals.

**4. Mössbauer Spectroscopy: (8 Hrs.)**

Experimental considerations, the spectrum and its parameters, simple spin states ( $I = 1/2, 3/2$ ), higher spin states ( $I > 3/2$ ), magnetic splitting significance of parameters obtained from spectra, quadruple splitting, additive model, interpretation of Mössbauer spectra of  $^{57}\text{Fe}$ ,  $^{119}\text{Sn}$ .

**5. Electron Paramagnetic Resonance Spectroscopy: (9 Hrs.)**

Introduction, principle, Presentation of spectrum, hyperfine splitting in isotropic systems involving more than one nucleus, esr spectrum of benzene radical anion, methyl radical.  $\text{CH}_2\text{OH}$  cyclopentadienyl cycloheptatrienyl radical, pyrazine anion, pyrazine anion with  $^{23}\text{Na}$  and  $^{39}\text{K}$  counter ion and Nitrosyl nitroxide, Factors affecting magnitude of g values, zero field splitting and Kramer's degeneracy.

Qualitative survey of EPR spectra of first row transition metal ion complexes ( $d^1, d^2, d^3$ , low spin  $d^5$ , high spin  $d^6, d^7, d^9$  system). Spectra of triplet states.

**Section C****6. X-ray Diffraction Methods of Analysis (9 hrs.)**

Production of X-rays, solid state symmetry, reciprocal lattice, Bragg's law in reciprocal space, the powder method, interpretation of powder pattern of a cubic system, particle size determination

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by powder method, qualitative and quantitative analysis using powder method. X-ray fluorescence spectroscopy, X-rays emission method, applications (qualitative and quantitative).

**7. Photoelectron Spectroscopy: (6 hrs)**

Introduction, photoelectron spectroscopy, chemical shift, X-ray photoelectron spectroscopy, molecular orbital diagrams of nitrogen and oxygen and their XPS spectra-ESCA, ultraviolet photoelectron spectroscopy (UPS), PES spectrum of nitrogen sample, vibrational structure in the N<sub>2</sub> UPS spectrum, chemical shifts in XPS, exchange splitting and shake up process

**Course Outcomes:**

CO1	MCHE-1204.1	The subject offers the readers a fundamental understanding of the spectroscopic techniques and their application for structure elucidation of organic molecules
CO2	MCHE-1204.2	To acquire knowledge of rotational vibrational, UV-VISIBLE, Massbauer, Xray diffraction and photoelectron spectroscopy and their applications
CO3	MCHE-1204.3	Basic understanding of IR, Raman, ESR, Mossbauer,
CO4	MCHE-1204.4	To understand the recent advancement of spectroscopic techniques used in the organic chemistry

**Books Recommended:**

1. R. S. Drago, "Physical Methods in Chemistry". W.B. Saunders Company.
2. C. N. Banwell "Fundamentals of Molecular Spectroscopy".
3. R. V. Parish, NMR, NQR, EPR & Mossbauer spectroscopy in Inorganic Chemistry. Ellis Horwood, London, 1990.
4. G. M. Barrow "Introduction to Molecular Spectroscopy".
5. E. A. Ebsworth, S.Craddock and D.W. H. Rankin, Structural methods in Inorganic Chemistry, Blackwell Scientific Publications (1991).
6. C.N.R. Rao and J.R. Ferraro, Spectroscopy in Organic Chemistry, Vol. I, Academic Press, 1971.

**SUBJECT TITLE: Bioorganic and Medicinal Chemistry****SUBJECT CODE: MCHE-1205****SEMESTER: II****CONTACT HOURS/WEEK:**

Lecture (L)	Tutorial (T)	Practical (P)	Credit (C)
3	0	0	3

**Internal Assessment: 40****End Term Exam: 60****Duration of Exam: 3 Hrs****Course Objective:** To impart advanced knowledge of enzymes, enzyme action and drug design**Section A****1. Enzymes: (8 Hrs)**

Basic considerations. Proximity effects and molecular adaptation. Introduction and historical perspective, chemical and biological catalysis, remarkable properties of enzymes like catalytic power, specificity and regulation. Nomenclature and classification, extraction and purification. Fischer's lock and key and Koshland's induced fit hypothesis, concept and identification of active site by the use of inhibitors, affinity labelling and enzyme modification by site-directed mutagenesis. Enzyme kinetics, Michaelis-menten and Lineweaver-Burk plots, reversible and irreversible inhibition.

**2. Mechanism of Enzyme Action: (5Hrs)**

Transition-state theory, orientation and steric effect, acid-base catalysis, covalent catalysis, strain or distortion. Examples of some typical enzyme mechanisms for chymotrypsin, ribonucleases, lysozyme and carboxypeptidase A.

**Section B****3. Kinds of Reaction Catalysed by Enzymes: (8Hrs)**

Nucleophilic displacement on a phosphorus atom, multiple displacement reaction and the coupling of ATP cleavage to endergonic processes. Transfer of sulphates, addition and elimination reactions, enolic intermediates in isomerization reactions,  $\beta$ -cleavage and condensation, some isomerisation and rearrangement reactions. Enzyme catalyzed carboxylation and decarboxylation.

**4. Co-Enzyme Chemistry: (6Hrs)**

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Cofactors as derived from vitamins, coenzymes, prosthetic groups, apoenzymes. Structure and biological function of coenzyme A, thiamine pyrophosphate, pyridoxal phosphate, NAD<sup>+</sup>, NADP<sup>+</sup>, FMN, FAD, LIPOIC ACID, vitamin B<sub>12</sub>. Mechanisms of reactions catalysed by the above cofactors.

**Section C**

**5. Drug Design: (18Hrs)**

Development of new drugs, procedures followed in drug design, concepts of lead compound and lead modification, concepts of prodrugs and soft drugs, structure-activity relationship (SAR), factors affecting bioactivity, resonance, inductive effect, isosterism, bio-isosterism, spatial considerations. Theories of drug activity: occupancy theory, rate theory, induced fit theory. Quantitative structure activity relationship. History and development of QSAR. Concepts of drug receptors. Elementary treatment of drug receptors interactions. Physico-chemical parameters: lipophilicity, partition coefficient, electronic ionization constants, steric, Shelton and surface activity parameters and redox potentials.

**Course Outcomes:**

CO1	MCHE-1205.1	To provide exposure of various biomolecules containing metal ions that comprises many important proteins and enzymes
CO2	MCHE-1205.2	Supramolecular chemistry of life. This course would be highly beneficial for students who had minimal exposure of bioinorganic chemistry at the undergraduate level.
CO3	MCHE-1205.3	To impart advance knowledge of enzymes and metal ions in biological systems
CO4	MCHE-1205.4	To impart the knowledge of biochemistry in daily life

**Books Recommended:**

1. Principles of Biochemistry By Lehninger
2. Principles of Biochemistry By Voet and Voet
3. The organic chemistry of drug design and drug action By R. B. Silverman, 2nd Ed., 2004, Academic press
4. An introduction to drug design by S. S. Pandeya and J.R. Dimmock, New Age International

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**SUBJECT TITLE: Organic Chemistry Lab-I****SUBJECT CODE: MCHE-1206****SEMESTER: II****CONTACT HOURS/WEEK:**

Lecture (L)	Tutorial (T)	Practical (P)	Credit (C)
0	0	6	3

**Internal Assessment: 40****End Term Exam: 60****Duration of Exam: 3 Hrs****Course Objective:** To teach the synthesis of organic compounds .

- 1 Prepare a sample of Ibuprofen
- 2 Preparation of oil of Wintergreen from commercial aspirin tablets
- 3 Nitration of o-chlorobenzoic acid and o-chloroacetanilide –separation and identification of isomers
- 4 Preparation of bromohydrin of  $\alpha$ - methylstyrene
- 5 Dihydroxylation of cyclohexene with peracids and  $\text{KMnO}_4$  –Product distribution by TLC
- 6 Preparation of carbene complex of Silver(I)Chloride
- 7 Solvent free Cannizzaro reaction using p-nitrobenzaldehyde
- 8 Synthesis of 1,1-diphenylethanol from phenyl magnesium bromide and acetophenone
- 9 Reduction of 3- nitroacetophenone using i)  $\text{NaBH}_4$  ii) using Sn and HCl.
- 10 Synthesis of N,N-diethylm-toluamide (mosquito repellent) from m-toluic acid
- 11 Synthesis of Aspirin, its mode of action and molecular modeling with cyclooxygenase
- 12 Isolation of essential oils from Caraway seeds and orange peels – (S) – Carvone and (R) - Limonene
- 13 Synthesis of styrene epoxide and ring opening reactions under neutral and acidic conditions
- 14 Diels – Alder reaction of a Danishefsky diene
- 17 Synthesis and oxidation of 1-aminobenzotriazole – Benzyne trapping



**Course Outcomes:**

CO1	MCHE-1206.1	To impart knowledge of Multi-step Synthesis in organic chemistry.
CO2	MCHE-1206.2	To provide the basics concept in Organic Chemistry at the beginning of the semester.
CO3	MCHE-1206.3	This course imparts purification methods, chromatographic separation and identification of organic compounds, solvent drying and functional group detection in organic compounds
CO4	MCHE-1206.4	Students would be familiarized with quantitative analysis of organic compounds to estimate the percentage of given functional groups.

**Books Recommended:**

1. Vogels's Textbook of Practical Organic Chemistry, 5th Edition ELBS (Longman), 1996.
2. Practical Organic Chemistry by F.G. Mann and B.C. Saunders, 5th Edition, Orient Longman Limited, 1986.

Program Code: MCHE-401

**SUBJECT TITLE: Electroanalytical Chemistry Lab****SUBJECT CODE: MCHE-1207****SEMESTER: II****CONTACT HOURS/WEEK:**

Lecture (L)	Tutorial (T)	Practical (P)	Credit (C)
0	0	6	3

**Internal Assessment: 40****End Term Exam: 60****Duration of Exam: 3 Hrs****Course Objective:** To teach the various analytical techniques**A. Conductometry**

1. Find graphically the equivalent conductance at infinite dilution of weak acid (benzoic acid, succinic acid, acetic acid) and hence determine the thermodynamic dissociation constant of the weak acid.
2. Determine the equivalent conductance of strong electrolytes ( $\text{KNO}_3$ ,  $\text{KCl}$ ) at several concentrations of its aqueous solution and verify the Onsager's equation.
3. Determine the equivalent conductance at infinite dilution of weak electrolytes ( $\text{CH}_3\text{COOH}$ ,  $\text{NH}_4\text{OH}$ ) in their aqueous solutions using Kohlraush law.
4. To determine relative strength of monochloroacetic and acetic acid by conductance measurements.

**B. Potentiometry and pHmetry**

5. To determine the dissociation constant of a dibasic acid (malonic acid)
6. The potentiometric titration of a mixture of Chloride and Iodide with  $\text{AgNO}_3$ .
7. To determine the degree of hydrolysis of aniline hydrochloride and hence hydrolysis constant of the salt.
8. Determination of acid and basic dissociation constants of an amino acid and hence the iso-electric point of the acid.
9. Titration of Phosphoric acid solution with  $\text{NaOH}$  using quinhydrone electrode.
10. The Potentiometric Determination of Solute Species in a Phosphate Mixture
11. The Potentiometric Titration of Copper with EDTA.

**C. Electrogravimetry and Coulometric Titrations**

12. Determination of Copper and Lead in a given sample of Brass Electrogravimetrically.
13. Determine coulometrically the concentration of Nickel and Cobalt from a given mixture.
14. The coulometric titration of cyclohexene.

**Course Outcomes:**

CO1	MCHE-1207.1	To impart knowledge of instruments and analytical tools used in chemistry.
CO2	MCHE-1207.2	To provide students exposure of pHmetry, potentiometry and conductometry experiments
CO3	MCHE-1207.3	At the end of this course students will be equipped to carry out instrumental analysis at the research level.
CO4	MCHE-1207.4	To develop the skill development knowledge based on instrumentation.

**Books Recommended:**

1. Findlay's Practical Physical Chemistry.
2. Advanced Practical Physical Chemistry by J.B. Yadav.



Program Name: Masters in Chemistry

Program Code: MCHE-401

## **SEMESTER III**

**SUBJECT TITLE: Inorganic Chemistry-III (Radiochemistry & Nanochemistry)****SUBJECT CODE: MCHE-2301****SEMESTER: III****CONTACT HOURS/WEEK:**

Lecture (L)	Tutorial (T)	Practical (P)	Credit (C)
3	0	0	3

**Internal Assessment: 40****End Term Exam: 60****Duration of Exam: 3 Hrs****Course Objective:** To impart advance knowledge of advance topics of inorganic chemistry**Section-A****1. Radiochemistry: (15 hrs)**

Discovery of radioactivity, statistical aspect of radioactivity, radioactive decay and growth, naturally occurring radioactive substances, nuclear structure and properties, nuclear reactions, nature of nuclear reactions, comparison of nuclear and chemical reactions, energetics of nuclear reactions, the Q-value of a reaction, Cross sections – partial reactions and total cross reaction. Bohr theory of nuclear reactions, types of reactions, Oppenheimer Phillips process, Photonuclear reactions, nuclear fission and fusion, fission products and fission yields, chain reaction at very high energies, nuclear transparency, high energy fission, slow neutron reactions Cross-section, equations of Radioactive decay and growth, equations of transformation in a neutron flux, gamma transitions and Isomerism, &  $\beta$  decay, Interaction of radiations with matter.

**Section-B****2. Traces in Chemical Applications: (8hrs)**

Isotopic and exchange reactions, qualitative observations, quantitative exchange law, reaction kinetics and mechanism, electron transfer reaction, rates of isotopic reactions

**3. Analytical Applications: (8hrs)**

Tests of separation, Analysis of Isotope dilution, health and safety aspects radio toxicity hazard, design features of the laboratories and their classifications, operational procedures and practices, radiation protection, radioactive and waste management, objective and principles.

**Section-C**

**4. Advanced Inorganic Materials: (10hrs)**

Nanotechnology and its business applications, Introduction to nanoscale, Potential applications of nanomaterials, Challenges and opportunities scope of nanotechnology, Commercialization scope Nanotechnology research in 21st century, Basic nanotechnology science and chemistry concepts, basic nanostructures, nanocomposites, Thin films, nanofoam, nanoclusters, smart nanostructures, manufacturing techniques of nanomaterials.

**5. Glass, Ceramics, Refractory materials: (4 hrs)**

Glassy states, Glass formers and glass modifiers, applications, ceramic structures, mechanical properties, clay products, refractory characterization, properties

**Course Outcomes:**

CO1	MCHE-2301.1	To impart advance knowledge of uses of Radiochemistry
CO2	MCHE-2301.2	Understand reaction mechanism and kinetics of isotopic and exchange reactions.
CO3	MCHE-2301.3	Explain various analytical reactions.
CO4	MCHE-2301.4	Explain cause and facture factors of Nanotechnology and its applications

**Books Recommended:**

1. Wilcox: Preparation and Properties of Solid State Materials: Vol I & II, Dekker
2. Solid State Chemistry: A.H. Hanny
3. Nuclear and Radiations Chemistry by Fiedelander and Kennedy.
4. Principles of Radio Chemistry, Indian Association of Nuclear Chemists and Allied Scientists  
Editors D.D. Sood, N. Rama moorthy, A.V.R. Reddy.

**SUBJECT TITLE: Organic Chemistry-III (Photochemistry & Pericyclic Reactions)****SUBJECT CODE: MCHE-2302****SEMESTER: III****CONTACT HOURS/WEEK:**

Lecture (L)	Tutorial (T)	Practical (P)	Credit (C)
3	0	0	3

**Internal Assessment: 40****End Term Exam: 60****Duration of Exam: 3 Hrs**

**Course Objective:** To impart advance knowledge of photochemical reactions, photochemistry of alkenes, carbonyl compounds, isomerization and photo fragmentation process

#### Section-A

##### 1. Photochemical Reactions: (4 Hrs)

Interaction of electromagnetic radiation with matter, types of excitations, fate of excited molecule, quantum yield, transfer of excitation energy,

##### 2. Determination of Reaction Mechanism: (4 Hrs.)

Classification, rate constants and life times of reactive energy states – determination of rate constants of reactions. Effect of light intensity on the rate of photochemical reactions

##### 3. Photochemistry of Alkenes: (6 Hrs.)

Intramolecular reactions of the olefinic bond- geometrical isomerism, cyclisation reactions, rearrangement of 1, 4-dienes,

#### Section-B

##### 4. Photochemistry of Carbonyl Compounds: (6 Hrs)

Photochemistry of Carbonyl compounds: Norrish Type I and II, Intermolecular and Intramolecular hydrogen abstraction, Paterno-Buchi reaction,  $\alpha$  and  $\beta$ - cleavage reactions of cyclic and acyclic carbonyl compounds, Formation of oxetane and cyclobutane from  $\alpha$ ,  $\beta$  unsaturated ketones, Photo-rearrangement of enones, dienones, epoxyketones, Photo Fries rearrangement.

**5. Photochemistry of Aromatic Compounds: (4 Hrs)**

Isomerisations, additions and substitutions.

**Section-C**

**6. Cycloadditions: (11 hrs.)**

Intermolecular [2+2] cycloadditions of alkenes and conjugated dienes, Photosensitised intermolecular cycloadditions of conjugated dienes, Photosensitised cyclodimerisation of 1, 3-Dienes, [2+2] photocycloaddition reactions of carbonyl compounds.

**7. Isomerisations and Rearrangements: (6 hrs.)**

Photochemical cis-trans isomerisation of alkenes, Photochemical cis-trans isomerisation of conjugated dienes, cis-trans isomerisation of cycloalkenes, Photovalence isomerisation reactions of benzene : Photochemistry of benzene valence Isomers, Photorearrangements of 2, 4-cyclohexadienones, Sigmatropic isomerisations of  $\beta$ ,  $\gamma$  - unsaturated enones, Photo-Fries rearrangement, Photo-Fries reactions of anilides, Barton reaction. Singlet molecular oxygen reactions

**9. Pericyclic Reactions: (8 hrs)**

Molecular Orbital symmetry, Frontier Orbitals of ethylene, 1,3 - butadiene, 1, 3, 5-hexatriene and allyl system. Classification of Pericyclic reactions. Woodward-Hoffman rule, correlation diagrams. FMO and PMO approach. Electrocyclic reactions - conrotatory and disrotatory motions  $4n$ ,  $4n+2$  and allyl systems. Cycloadditions - antarafacial and suprafacial additions  $4S+2S$  Systems and  $2S+2S$  additions of alkene. Sigmatropic rearrangement - suprafacial and antarafacial shift involving carbon moieties. 3, 3- and 5, 5-sigmatropic rearrangement Claisen, Cope-rearrangement reactions.

**Course Outcomes:**

CO1	MCHE-2302.1	Understand the basic concept of organic chemistry.
CO2	MCHE-2302.2	To impart advance knowledge synthesis of organic compounds and organic reactions.
CO3	MCHE-2302.3	Describe and demonstrate the importance of molecular rearrangements in organic compound synthesis and understand the basics of photochemistry and pericyclic reactions.



CO4	MCHE-2302.4	Describe the interaction of excited states with their surroundings and analyze photo-induced electron transfer/excitation energy transfer reaction.
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**Books Recommended:**

1. Fundamental of PhotoChemistry By K.K. Rohtagi Mukherji
2. Molecular Photochemistry By N.J. Turro and W.A. Benjamin
3. Introductory Photochemistry By A. Cox and T. Camp
4. Modern Organic Photochemistry By W. H. Horsepool
5. K. K. Rohatgi Mukherji, Fundamentals of Photochemistry, Reprint, Revised edition, New Age International (P) Ltd., Publishers, New Delhi, INDIA, 1997.
6. S. M. Mukherji, Pericyclic Reactions : A Mechanistic Study, The MacMillan Co. of India Ltd., New Delhi, INDIA, 1979.

Program Code: MCHE-401

**SUBJECT TITLE: Macromolecules and Surface Chemistry****SUBJECT CODE: MCHE-2303****SEMESTER: III****CONTACT HOURS/WEEK:**

Lecture (L)	Tutorial (T)	Practical (P)	Credit (C)
3	0	0	3

**Internal Assessment: 40****End Term Exam: 60****Duration of Exam: 3 Hrs****Course Objective:** To impart advance knowledge of polymers and their chemistry

### Section-A

#### 1. Macromolecule: (8 hrs)

Classification and nomenclature of polymers, composition and polymerization mechanism. regular and irregular polymers, electrically conducting polymers, physical properties of solid polymers (crystallinity, plasticity & elasticity) vulcanization of rubbers, polymer solutions, factors affecting the solubility of polymers.

### Section-B

#### 2. Step Polymerization: (8hrs)

Reactivity of functional groups, basis for analysis of polymerization, kinetics of step polymerization, self catalysed polymerization, external catalysis of polymerization, step polymerization other than polyesterification non-equivalence of functional groups in polyfunctional reagents.

#### 3. Radical chain polymerization: (10hrs)

Overall kinetics of chain polymerization, initiation, thermal decomposition of initiators, types of initiators, kinetics of initiation and polymerization, dependence of polymerization rate on monomer, photochemical initiation, initiation by ionizing radiation, pure thermal initiation, redox initiation.

### Section-C

#### 4. Co-polymerization and emulsion polymerization: (6hrs)

## Program Code: MCHE-401

The composition of addition copolymers, kinetics of chain propagation in co-polymerization, qualitative and quantitative theories of emulsion. Polymerization rate, degree and number of polymer particles in emulsion polymerization.

**5. Molecular weight: (5hrs)**

Average and viscosity average molecular weight, molecular weight determination by osmotic method, light scattering method, sedimentation method, diffusion constant, sedimentation equilibrium, viscosity method, ultracentrifuge methods.

**6. Statistics of Linear polymers: (5hrs)**

Molecular weight, molecular weight distribution, polydispersity, index, average and end to end distance, average radius of gyration.

**Course Outcomes:**

CO1	MCHE-2303.1	Understand the basics of polymers, electric behavior, composition, and solubility
CO2	MCHE-2303.2	Understand the reactivity and analysis of polymerization and significance of functional groups
CO3	MCHE-2303.3	Understand the mechanism and kinetics of polymerization and determination of molecular weights and their methods
CO4	MCHE-2303.4	Understand the basic Statistics involve in the Linear polymers

**Books Recommended:**

1. Principles of Polymerization by George Odian.
2. Principles of Polymer Chemistry by Paul J. Flory.
3. Text book of Physical Chemistry by Glastone.
4. Physical Chemistry of Macromolecules by Charles Tanford.
5. Physical Chemistry by G. M. Barrow

**SUBJECT TITLE: Spectroscopy in Structure Elucidation and Asymmetric Synthesis****SUBJECT CODE: MCHE-2304****SEMESTER: III****CONTACT HOURS/WEEK:**

Lecture (L)	Tutorial (T)	Practical (P)	Credit (C)
4	0	0	4

**Internal Assessment: 40****End Term Exam: 60****Duration of Exam: 3 Hrs**

**Course Objective:** To impart advance knowledge of Asymmetric Synthesis, Organocatalysis in Organic Synthesis, spectroscopic techniques and their application

### Section-A

#### 1. Asymmetric Synthesis: (15 Hrs)

Analytical methods for determination of enantiomeric purity – GC, HPLC and NMR. Natural sources of chiral starting materials, classification and methods of formation of new chiral compounds.

##### **Non-enzymatic Approaches:**

Methods of asymmetric synthesis using naturally occurring chiral compounds, nucleophile and electrophile bearing chiral auxiliary, Diels – Alder cycloaddition and Claisen – cope rearrangements.

Asymmetric carbon – carbon bond formation using alkylation, Michael reaction and addition to carbonyl compounds. Cram's rule and Felkin – Ahn model. Asymmetric oxidation and reductions.

##### **Enzymatic Approaches:**

Enzymatic and Microbial methods in asymmetric synthesis. Use of different types of enzymes lipases, oxidases etc. in organic synthesis.

### Section-B

#### 2. Organocatalysis in Organic Synthesis: (8 Hrs)

Program Code: MCHE-401

Introduction. Enamine catalysis: Aldol and Mannich type reactions,  $\alpha$ -heteroatom functionalization, direct conjugate additions via enamine activation. Iminium catalysis: the catalysis concept, cycloaddition reactions, 1,4-addition reactions, transfer hydrogen, cascade reactions. Ammonium ions as chiral templates: Homogeneous catalysis with chiral quaternary ammonium salts, Heterogeneous catalysis- chiral phase transfer catalysis. Morita-Baylis-Hillman reaction: addition of ketones and aldehydes to activated olefins, asymmetric MBH reactions.

**Section-C**

**Asymmetric proton Catalysis: (7 Hrs)**

conjugate addition reactions, hydrocyanation reactions, mannich reactions, aza-henry reaction, acyl Pictet-Spengler reaction, aza Friedel-Crafts reaction. Chiral Lewis bases as catalysts: allylation reactions, propargylation reactions, hydrocyanation and isonitrile addition, aldol type reactions, reduction of imines, epoxide ring opening. Asymmetric acyl transfer reactions. Nucleophilic N-Heterocyclic carbenes. Ylide based reactions. Organocatalytic oxidations and reduction reaction

**3. The applications of spectroscopic techniques in structure elucidation: (15 Hrs)**

**Introduction to FT NMR**

<sup>13</sup>C NMR, normal and DEPT spectra and their applications in structure elucidation. Use of <sup>1</sup>H NOE in analysis of geometry in three, four and five member rings and double bonds. To discuss the problems by using UV- VIS , I.R., Mass and NMR spectral data for the structure elucidation of organic molecules

**Course Outcomes:**

CO1	MCHE-2304.1	The subject offers the readers a fundamental understanding of the spectroscopic techniques and their application for structure elucidation of organic molecules
CO2	MCHE-2304.2	Understand UV- VIS, I.R., Mass and NMR spectral data for the structure elucidation of organic molecules
CO3	MCHE-2304.3	Explanation of Non-enzymatic Approaches: Methods of asymmetric synthesis using naturally occurring chiral compounds, nucleophile and electrophile bearing chiral auxiliary, Diels – Alder cycloaddition and Claisen – cope rearrangements.
CO4	MCHE-2304.4	To understand the recent advancement of spectroscopic techniques used in the organic chemistry

**Books Recommended:**

1. Structure Elucidation in Organic Chemistry: The Search for the Right Tools Maria-Magdalena Cid (Editor), Jorge Bravo (Editor)

Program Code: MCHE-401

**SUBJECT TITLE: Biochemistry Lab**

**SUBJECT CODE: MCHE-2305**

**SEMESTER: III**

**CONTACT HOURS/WEEK:**

Lecture (L)	Tutorial (T)	Practical (P)	Credit (C)
0	0	6	3

**Internal Assessment: 40**

**End Term Exam: 60**

**Duration of Exam: 3 Hrs**

**Course Objective:** To impart advance knowledge of Identification of Biomolecules.

- 1) Identification of biomolecules - Amino acids, proteins, carbohydrates, lipids.
- 2) Estimation of the strength of amino acid using formol titration
- 3) Separation of amino acids using paper chromatography
- 4) Separation of amino acids using thin layer chromatography (TLC)
- 5) Estimation of proteins using Folin Ciocalteu (Lowry) method.
- 6) Estimation of Vitamin-C using 2,6-dichlorophenol indophenol.
- 7) Estimation of soluble calcium in milk using EDTA.
- 8) Estimation of total phenolic content in Black Tea.
- 9). Determination of dissolved oxygen in water.
- 10). Determination of Chemical Oxygen Demand (COD)
- 11). Determination of Biological Oxygen Demand (BOD)
- 12) Percentage of available chlorine in bleaching powder

**Course Outcomes:**

CO1	MCHE-2305.1	To identify biomolecules - Amino acids, proteins, carbohydrates, lipids.
CO2	MCHE-2305.2	To separation of amino acids
CO3	MCHE-2305.3	Understanding of process of Estimation of proteins

CO4	MCHE-2305.4	Determination of Chemical Oxygen Demand (COD) and Biological Oxygen Demand (BOD)
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**Books Recommended:**

- (i) An Introduction to Practical Biochemistry – David T Plummer
- (ii) Introductory Practical Biochemistry – Sawhney & Sing
- (iii) Biochemical Methods – S. Sadasivam and A. Manickam
- (iv) Experimental Biochemistry - Rao & Deshpande



Program Code: MCHE-401

**Optional Subjects**  
**(Inorganic Chemistry)****SUBJECT TITLE: Coordination Chemistry****SUBJECT CODE: MCHE-2306****SEMESTER: III****CONTACT HOURS/WEEK:**

Lecture (L)	Tutorial (T)	Practical (P)	Credit (C)
3	0	0	3

**Internal Assessment: 40****End Term Exam: 60****Duration of Exam: 3 Hrs**

**Course Objective:** To impart advance knowledge of theories, reaction mechanism and stability of coordination complexes, magnetic and electronic properties.

**Section-A****1.Theories of Metal-Ligand bonding: (6 hrs)**

Molecular Orbital treatment, Octahedral (with and without pi bonding) tetrahedral and square planer complexes in a qualitative manner, comparison of theories of bonding, VBT, CFT, LFT and MOT.

**2.Structural studies of coordination compounds: (6 hrs)**

Compounds of first transition series elements, with respect to their electronic spectra, magnetic & thermal properties (DTA, TGA)

**Section-B****3.Magneto Chemistry: (8 hrs)**

Diamagnetic correction, single & multielectron system, types of the magnetic behaviour, Diamagnetism, Para magnetism, Ferro & Ferri, Antiferro and magnetic interaction, The origin of Para magnetism, Magnetic behavior of complexes, Simplification of Van Velck equation, magnitude of magnetic moments, Determination of magnetic susceptibility by Gouy and faraday method.

**4.Transition metal complexes & catalysis: (8 hrs)**

Program Code: MCHE-401

Introduction, General Principle, catalysis by transition metal complexes, Hydrocarbons Oxidation by Molecular oxygen, olefin Oxidation, olefin polymerization, olefin hydrogenation, Arene reactions catalyzed by metal complexes, catalysis of condensation polymerization reaction, Current and feature trend in catalysis.

**Section-C**

**5.Mixed Ligand complexes: (7 hrs)**

Stabilities of ternary complexes, Dynamics of formation of ternary complexes reaction of Coordination ligand in ternary complexes, Mimicking reactions in biological systems, enzyme models, Amino acids ester hydrolysis, peptide synthesis & hydrolysis, Detarbodylation of B keto acids

**6.Structures of Important Complexes: (10 Hrs)**

Structure of some important complexes of the first transition series (to be discussed in terms of coordination number, shape or oxidation states or nature of bonding),  $Ti(NO_3)_4$ ,  $TiCl_4(diams)_2$ ,  $[Ti(Oet)_4]_4$ ,  $VF_5$ ,  $VO(acac)_2$  and nature of  $VO_2^+$  bond,  $[VOCl_3(NMe_3)_2]$ ,  $CrO_4^{2-}$ ,  $Cr_2O_7^{2-}$   $[CrO(O_2)_2 Py]$ ,  $[Cr(O_2)_2(bipy)]$ , nature of metal, peroxo bond,  $Cr_2(2- acetate)_4$  and the nature of Cr-Cr bond in this complex, tetrameric  $[Co(acac)_2]_4$ , tetrahedral complexes being more common in case of cobalt, oxidation of Co(II), complexes by molecular  $O_2$ ,  $[Ni(acac)_2]_3$ ,  $Ni(DMGH)_2$ ,  $[Ni(Me_6 - acac)_2]$ ,  $[Ni(MeSal)_2]$ ,  $[Ni(CN)_5]^{3-}$ , anomalous behaviour of nickel(II) complexes, copper(II) acetate dihydrate,  $[Cu(CN)_2]^{2-}$ , cubane complexes  $[CuXL]_4$  where X=halide and L=phosphine or arsine.

**Course Outcomes:**

CO1	MCHE-2306.1	To impart advance knowledge of theories of Metal-Ligand bonding
CO2	MCHE-2306.2	Understand reaction mechanism and kinetics of reaction mechanism and stability of coordination complexes.
CO3	MCHE-2306.3	Explain magnetic and electronic properties of transition metal complexes
CO4	MCHE-2306.4	Explain cause and facture factors of Transition metal complexes & catalysis

**Books Recommended:**

1. Jones: Elementary Coordination Chemistry. J. Wiley

## Program Code: MCHE-401

2. Graddon: Introduction to Coordination Chemistry. J. Weily
3. Drago: Physical methods of Inorganic Chemistry. J. Weily.
4. Graddon: Introduction to coordination Chemistry, Parasmom
5. Lewis and Wilkins: Coordination Chemistry. J. Weily
6. Msrtel: Coordination Chemistry Vol I, II VNR
7. Earnshaw: Introduction to Magneto Chemistry
8. Mabbs & Machin Magnetism & transition metal complexes Chamman hall
9. Calvin, Magnetic properties of transition metal complexes.
10. L.N. Maley: Magneto Chemistry
11. Datta & Shymal Elements of Magneto Chemistry
12. Martel & Taqui Khan: homogeneous catalysis with metal complexes Vol.I & II AP.
13. James E. Huheey: Inorganic Chemistry Principles of Structure and reactivity, Harber & Row, Publishers Inc. New York 1972.
14. K.P. Purcell & J.C. Kote: An Introduction to Inorganic Chemistry Holt Sounders, Japan 1980.
15. William L. Jolly: Modern Inorganic Chemistry, Mecgrow Hill USA,1984
16. F.A. Cotton & R.G. Wilkinson: Advanced Inorganic Chemistry.

**SUBJECT TITLE: Nuclear Chemistry****SUBJECT CODE: MCHE-2307****SEMESTER: III****CONTACT HOURS/WEEK:**

Lecture (L)	Tutorial (T)	Practical (P)	Credit (C)
3	0	0	3

**Internal Assessment: 40****End Term Exam: 60****Duration of Exam: 3 Hrs****Course Objective:** To impart advance knowledge of nuclear phenomenon**Section-A****1. Systematic of alpha, beta and gamma decays: (8 Hrs)**

Alpha decay, energy curve, spectra of alpha particles, Giger-Nuttal law, theory of alpha decay, penetration of potential barrier, beta decay, range of energy relationship, beta spectrum, sergeants curve, Fermi theory of beta decay, matrix elements, allowed and forbidden transitions, curie plots, gamma decay, Nuclear energy levels, selection rule, isomeric transitions, Internal conversion, Auger effect.

**2. Nuclear Structure and Stability: (8 Hrs)**

Binding energy, empirical mass equation, The nuclear models, the liquid drop model, the shell model, the Fermi gas model & collective nuclear model, nuclear spin, parity & magnetic moments of odd mass numbers nuclei.

**Section-B****3. Nuclear reaction: (8 Hrs)**

Introduction, Production of projectiles, nuclear cross section, nuclear dynamics, threshold energy of nuclear reaction, Coulomb scattering, potential barrier, potential well, formation of a compound nucleus, Nuclear reactions, direct Nuclear reactions, heavy ion induced nuclear reactions, photonuclear reactions.

**4. Nuclear fission: (6 Hrs)**

## Program Code: MCHE-401

Liquid drop model of fission, fission barrier and threshold, fission cross section, mass energy and charge distribution of fission products, symmetric and A symmetric fission, decay chains and delayed neutrons.

**Section-C****5. Reactor Theory: (9 Hrs)**

Nuclear fission as a source of energy, Nuclear chain reacting systems, critical size of a reaction, research reactors, graphite moderated, heterogeneous, enriched uranium reactors, light water moderated, heterogeneous, enriched uranium reactors, water boilers enriched aq. Homogeneous reactors, Thermonuclear reactors, gamma interactions, shielding and health protection. Reactors in India.

**6. Nuclear Resources in India: (6 Hrs)**

Uranium and Thorium resources in India and their extractions, Heavy water manufacturing in India.

**Course Outcomes:**

CO1	MCHE-2307.1	To impart advance knowledge of nuclear phenomenon
CO2	MCHE-2307.2	Understand reaction mechanism and kinetics of reaction mechanism and stability of Nuclear reaction.
CO3	MCHE-2307.3	Understand the basic concept of Nuclear Structure and Stability
CO4	MCHE-2307.4	Provide an overview of field of nuclear fission

**Books Recommended**

1. B.C. Harvey, Introduction to Nuclear Chemistry, Prentice-Hall (1969)
2. G. Friedlander, J.W. Kennedy, E.S. Marcus & J.M. Miller Nuclear & Radiochemistry. John-Wiley & Sons (1981)

**SUBJECT TITLE: Inorganic Chemistry Lab– II**
**SUBJECT CODE: MCHE-2308**
**SEMESTER: III**
**CONTACT HOURS/WEEK:**

Lecture (L)	Tutorial (T)	Practical (P)	Credit (C)
0	0	6	3

**Internal Assessment: 40**
**End Term Exam: 60**
**Duration of Exam: 3 Hrs**

**Course Objective:** To impart advance knowledge of spectroscopic techniques.

**Synthesis & study of IR Spectroscopy**

Study of the following complexes.

- (i)  $[\text{Co}(\text{NH}_3)_5\text{NO}_2]\text{Cl}$
- (ii)  $[\text{Co}(\text{NH}_3)_5\text{ONO}]\text{Cl}$
- (iii)  $[\text{Cr}(\text{urea})_6]\text{Cl}_2$
- (iv) Na diethyldithiocarbamate.

I. Determination of stoichiometry of complex of Fe - 1,10 - Phenanthroline by (a) Job's method of continuous variation. (b) Mole-Ratio Method.

II. To find out oscillator strength and assignments of d-d bands to transitions hexaquo ions of Cr (III), Fe (II), Ce (III), Co (II) and Ni (II). (c) Calculation of  $10 Dq$  and  $\beta$  for hexa aquo ion of Ni (II). (d) Verification of relative positions of following ligands in the spectrochemical series:  $\text{H}_2\text{O}$ , Py,  $\text{NH}_3$ , DMSO, Acetyl acetonate, ethylenediamine, acetate and urea.

**Course Outcomes:**

CO1	MCHE-2308.1	To impart basic knowledge of spectroscopic techniques
CO2	MCHE-2308.2	Understand Synthesis of inorganic complexes
CO3	MCHE-2308.3	Understand and study of IR Spectroscopy of inorganic complexes

CO4	MCHE-2308.4	Determination of stoichiometry of complex of Job's method of continuous variation and Mole-Ratio Method
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**Books Recommended:**

3. Vogel's book on Inorganic Qualitative Analysis 6<sup>th</sup> Edition
4. Vogel's book on Inorganic Quantitative Analysis 6th Edition

**Optional Subjects (Organic Chemistry)****SUBJECT TITLE: Stereochemistry: Conformation and mechanism****SUBJECT CODE: MCHE-2309****SEMESTER: III****CONTACT HOURS/WEEK:**

Lecture (L)	Tutorial (T)	Practical (P)	Credit (C)
3	0	0	3

**Internal Assessment: 40****End Term Exam: 60****Duration of Exam: 3 Hrs**

**Course Objective:** To impart advance knowledge stereochemistry of organic compounds and organic reactions.

**Section A****1. Chirality: (10 Hrs)**

Isomers and stereoisomer, configurations and their specifications, representation of three dimensional molecules, interconversion between fisher and three dimensional formulas, symmetry elements, resolution of racemic mixture (Resolution of acids, bases, amino acids, alcohols, aldehydes and ketones) Absolute and Relative configuration. Assymmetric induction , racemic mixture and racemization, stereoselective and stereospecific reactions, enantiomeric excess, nomenclature of compounds with axial chirality.

**2. Prochirality: (5 Hrs)**

Homotopic and heterotopic ligands faces, nomenclature of heterotopic ligands and faces and some streoselective reactions, Asymmetric synthesis, principle of categories of asymmetric synthesis, use of chiral reagents.

**Section B****3. Asymmetric synthesis: (7 Hrs)**



Program Code: MCHE-401

Principle of categories of asymmetric synthesis, use of chiral reagents, phase transfer catalysis. phase transfer catalysis

**4. Aliphatic nucleophilic substitution: (8 Hrs)**

Introduction,  $SN^2$  reaction mechanism and evidence,  $SN^1$  reaction, Nucleophilic substitution of allylic systems, at benzylic position, at vinylic and aryl halides, nucleophilic displacements at allylic halides,  $SNi$ ,  $SN^1$  and  $SN^2$  reactions. Set Mechanism and anchimeric assistance.

**Section C**

**5. Stereochemistry of elimination reactions: (8 Hrs)**

Introduction, Mechanisms E1, E2, and E1cB and their mechanistic spectrum, comparison between elimination and substitution, Stereochemistry of E2 anti and syn elimination reactions, regiochemistry of the elimination reactions, Pyrolytic elimination reactions Pyrolysis of acetate, Xanthates and amine oxide, fragmentation reaction reactions.

**6. Addition of organometallic compounds to carbon hetero multiple bonds: (7 Hrs)**

Grignard reagent to aldehyde and ketones, Gilman reagent, organo zinc compounds, Wittig reactions.

**Course Outcomes:**

CO1	MCHE-2309.1	The subject offers the readers a fundamental understanding of the stereochemistry of organic compounds
CO2	MCHE-2309.2	Understand To impart advance knowledge stereochemistry organic reactions and data for the structure elucidation of organic molecules
CO3	MCHE-2309.3	Explain Asymmetric synthesis And Aliphatic nucleophilic substitution
CO4	MCHE-2309.4	To understand the recent advancement of Addition of organometallic compounds to carbon hetero multiple bonds

**Books Recommended:**

1. Stereochemistry of Carbon Compounds by Ernest, L. Eliel, Tata McGraw-Hill.
2. Stereochemistry of Organic Compounds, D. Nasipuri, New Age International.

3. Stereochemistry of Organic Compounds, P.S. Kalsi, New Age, International.
4. Modern Organic Reactions, H.C. House, Benjamin.

**SUBJECT TITLE: Organic Synthesis-IV****SUBJECT CODE: MCHE-2310****SEMESTER: III****CONTACT HOURS/WEEK:**

Lecture (L)	Tutorial (T)	Practical (P)	Credit (C)
3	0	0	3

**Internal Assessment: 40****End Term Exam: 60****Duration of Exam: 3 Hrs**

**Course Objective:** To impart advance knowledge synthesis of organic compounds and organic reactions.

#### **Section-A**

##### **1. An introduction of synthesis and synthetic equivalents: (16 hrs)**

General principle of disconnection approach; Importance of order of event in organic synthesis. Introductory meaning of one CX and two C-X groups disconnection. Reversal of polarity (umpolung) New application of organosilicene compounds, cyclisation reactions of carbene and nitrenes. Protective Groups : Principle of protection of alcoholic amino carbonyl and carboxylic groups with suitable examples from synthetic point of view.

Synthesis of alkene,  $\beta$  – elimination pyrolytic syn elimination, synthesis of allyl alcohol, sulphoxide sulphenate rearrangement, through phosphorous ylid, decarboxylation of  $\beta$  – lactum stereo selective synthesis of tri-tetra substituted alkenes through use of acetylenes. Use of nitro compounds in organic synthesis. Fragmentation of sulphonates, oxidative decarboxylation of carboxylic acids. Decomposition of toluene p-sulphonylhydrazones, stereospecific synthesis from – 1,2-diols. Stereoselective route to  $\gamma$ ,  $\delta$ –carbonyl compounds.

#### **Section-B**

##### **2. C-C bond formation: (14 hrs)**

Generation and importance of enolate ion, regioselectivity, stereoselectivity. Generation of dianion and their alkylation, alkylation of relatively acidic methylene groups. Hydrolysis and

## Program Code: MCHE-401

decarboxylation of alkylated product, O-Vs-C alkylation, C-alkylation of vinyl group, aryl group. Formation of enamines and alkylation. Alkylation of carbon by conjugate additions.

**3. One group C-C - disconnection:**

Disconnection of simple alcohols, of simple olefins, carbonyl compounds control in synthesis, friedal craft's type examples.

**Section-C (15hrs)****4. Reaction of carbon nucleophiles with carbonyl group :**

Condensation process favoured equilibrium by dehydration of aldol products, under acidic and basic conditions, Amine catalysed condensation, Mannich Reaction, Nucleophilic addition, Cyclisation process, Derzen, Perkin, Stobbe reaction. Sulphur slides, phosphorous ylides and related spices as nucleophiles.

**5. Diels Alder Reaction :**

General feature dienophile diene, intramolecular Diels Alder reaction stereochemistry and mechanisms, photo sentized Diels Alder Reaction, homo Diels Alder reaction, ene synthesis, cycloaddition reaction of allyl cations/anions. Retro-Diels Alder's Reaction.

**Course Outcomes:**

CO1	MCHE-2310.1	The subject offers the readers a fundamental understanding of synthesis and synthetic equivalents
CO2	MCHE-2310.2	To Understand Generation and importance of enolate ion, regioselectivity, stereoselectivity
CO3	MCHE-2310.3	Knowledge of Reaction of carbon nucleophiles with carbonyl group
CO4	MCHE-2310.4	Detailed analysis of Diels Alder Reaction

**Books Recommended:**

1. W. Carruther : Some Modern Method of Organic Synthesis.
2. H. O. House : Modern Synthetic Reactions.
3. I. L. Finar : Organic Chemistry, Vol.2.
4. R.O.C. Norman; J.M. Coxon : Principles of Organic Synthesis.

**SUBJECT TITLE: Organic Chemistry Lab-II**

**SUBJECT CODE: MCHE-2311**

**SEMESTER: III**

**CONTACT HOURS/WEEK:**

Lecture (L)	Tutorial (T)	Practical (P)	Credit (C)
0	0	6	3

**Internal Assessment: 40**

**End Term Exam: 60**

**Duration of Exam: 3 Hrs**

**Course Objective:** To impart advance knowledge synthesis of organic compounds and their analysis.

**1. Qualitative Organic Analysis:**

Separation and purification of components of binary mixture (Solid/solid, solid/liquid and liquid/liquid) on the basis of solubility behaviour and solvent extraction and their identification and conformation by chemical tests and preparation of suitable derivative. Preparative TLC separation for IR and PMR spectral studies of the respective component.

**2. Organic Synthesis Benzoylation :**

Hippuric acid Oxidation : Adipic acid/p-Nitrobenzoic acid Aldol condensation : Dibenzalacetone/Cinnamic acid Sandmeyer's reaction : p-Chlorotoluene Benzfused Heterocycles : Benzimidazole Cannizzaro's reaction : p-Chlorobenzaldehyde as substrate Friedel Crafts reaction : S-Benzoylpropionic acid Aromatic electrophilic substitution : p-Nitroaniline / p-Iodoaniline The products may be characterized by spectral techniques.

**Course Outcomes:**

CO1	MCHE-2311.1	To impart advance knowledge synthesis of organic compounds and their analysis
CO2	MCHE-2311.2	Understanding of Qualitative Organic Analysis
CO3	MCHE-2311.3	Understand the basic concept of Organic Synthesis Benzoylation

CO4	MCHE-2311.4	Synthesis of Benzfused Heterocycles
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**Books Recommended:**

1. Vogels's Textbook of Practical Organic Chemistry, 5th Edition ELBS (Longman), 1996.
2. Practical Organic Chemistry by F.G. Mann and B.C. Saunders, 5th Edition, Orient Longman Limited, 1986.

**Optional Subjects (Physical Chemistry)****SUBJECT TITLE: Chemistry of Materials****SUBJECT CODE: MCHE-2312****SEMESTER: III****CONTACT HOURS/WEEK:**

Lecture (L)	Tutorial (T)	Practical (P)	Credit (C)
3	0	0	3

**Internal Assessment: 40****End Term Exam: 60****Duration of Exam: 3 Hrs**

**Course Objective:** To acquire knowledge of different types of materials, their properties and applications

**Section-A****1. Multiphase Materials: (5 Hrs)**

Ferrous alloys; Fe-C phase transformation in ferrous alloys; stainless steels, non-ferrous alloys, properties of ferrous and non-ferrous alloys and their applications.

**2. Glasses, Ceramics, Composites and Nanomaterials: (8 Hrs)**

Glassy state, glass formers, and glass modifiers, application. Ceramic structures, mechanical properties, clay particle product. Refractories, characterization, properties, and applications. Microscopic composites; dispersion-strengthened and particle reinforced, fibre-reinforced composite, macroscopic composites. Nanocrystalline phase, preparation procedure, special properties, applications.

**Section-B****3. Thin Films and Langmuir-Blodgett Films: (6 Hrs)**

## Program Code: MCHE-401

Preparation techniques; evaporation/sputtering, chemical process, sol gel etc. Langmuir – Blodgett (LB) films, growth technique, photolithography, properties and applications of thin and LB films.

**4. Liquid Crystals: (8 Hrs)**

Mesomorphic behaviour, thermotropic liquid crystal, positional order, bond orientational order, nematic and smectic mesophases; smectic – nematic transition and clearing temperature homeotropic, planar and schlieren textures, twisted nematics, chiral nematics, molecular arrangement in smectic A and smectic C phases, optical properties of liquid crystal. Dielectric susceptibility and dielectric constants. Lyotropic phases and their description of ordering in liquid crystals.

**Section-C****5. High Tc Materials: (6Hrs)**

Defect perovskites, high Tc superconductivity in Cuprates, preparation and characterization of 1-2-3 and 2-1-4 materials, normal state properties; anisotropy; temperature dependence of electrical resistance; optical phonon modes, superconducting state; heat capacity; coherence length, elastic constants, position lifetime, microwave absorption-pairing and multigap structure in high Tc materials, applications of high Tc materials.

**6. Materials for Solid State Devices: (5 Hrs)**

Rectifiers, transistors, capacitors –IV-V compounds, low-dimensional quantum structure; optical properties.

**7. Organic Solid, Fullerenes, Molecular Devices: (7 Hrs)**

Conduction organics, organics, organic superconductors, magnetism in organic materials. Fullerenes- doped, fullerenes as superconductors.

Molecular rectifiers and transistors, artificial photosynthetic devices, optical storage memory, switches and sensors.

Nonlinear optical materials: nonlinear optical effects, second and third order – molecular hyperpolarisability and second order electric susceptibility – materials for second and third harmonic generation.



**Course Outcomes:**

CO1	MCHE-2312.1	To impart properties of ferrous and non-ferrous alloys and their applications
CO2	MCHE-2312.2	Understand of Glasses, Ceramics, Composites and Nanomaterials.
CO3	MCHE-2312.3	Understand the basic concept of Thin Films and Langmuir- Blodgett Films
CO4	MCHE-2312.4	Provide an overview of field of Liquid Crystals, High Tc Materials, Materials for Solid State Devices Organic Solid, Fullerenes, Molecular Devices

**Books Recommended:**

1. Solid State Physics, N.W. Ashcrofy and N.D. Mermin, Saunders College.
2. Material Science and Engineering, An Introduction, W.D. Callister, Willey.
3. Principle of the Solid State, H.V. Keer, Willey Eastern.
4. Material Science, J.C. Anderson, K.D. Leaver, J.M. Alexander and R.D. Rawlings, ELBS
5. Thermotropic Liquid Crystals, Ed., G.W. Gray, John Willey.

**SUBJECT TITLE: Physical Chemistry-III****SUBJECT CODE: MCHE-2313****SEMESTER: III****CONTACT HOURS/WEEK:**

Lecture (L)	Tutorial (T)	Practical (P)	Credit (C)
3	0	0	3

**Internal Assessment: 40****End Term Exam: 60****Duration of Exam: 3 Hrs**

**Course Objective:** To acquire knowledge of photo physical, electrochemistry and their applications.

### SECTION-A

#### 1. Principles and Concepts: (7 Hrs)

Laws of photochemistry, Atomic and molecular term symbols, Electronic transitions, Jablonski diagram and photophysical processes, Radiative transitions, Absorption and emission, Absorption coefficient, Phosphorescence, Intersystem crossing, Mechanisms of singlet-triplet conversion (spin-orbit coupling), Spin rephasing, Spin flip, Importance of electron jump between perpendicular orbital's, heavy atom effect, Examples of ISC between states of different configurations, Radiative rates, Radiationless transitions, Internal conversion, Energy gap law, Deuterium effect.

#### 2. Electronically Excited States: (7 Hrs)

Electronic, Vibrational and spin configurations, Excited state lifetime, Steady state and time resolved emission, Factors affecting excited state energy, Solvent effect, TICT, Origin of

## Program Code: MCHE-401

energy difference between singlet and triplet states, Excited state kinetics, Quantum yield expressions, Excimer and exciplex, Kinetics of luminescence quenching, Static and dynamic, SternVolmer analysis, Deviation from Stern-Volmer kinetics, Photoinduced electron transfer rates, Free energy dependence of electron transfer on rate, Photoinduced energy transfer, FRET, ESPIT, TBET, Rate and efficiency calculation of FRET.

**SECTION-B****3. Theory of Photoreactions: (5 Hrs)**

Visualization of reactions on excited state surfaces, Minima, Funnels and conical intersections.

**4. Identification of Minima on Excited State Surfaces: (5 Hrs)**

Surface touching, Cleavage of s and p bonds, Diradicals, Salem diagrams, Photochemical generation and excited state reactions of reactive intermediates (carbenes, nitrenes, radicals, diradicals, and carbocations).

**5. Applications of Photochemistry and Photophysical Principles: (6 Hrs)**

Measurement of fluorescence and phosphorescence and lifetimes, Introduction to time-resolved techniques for absorption and emission measurements, Detection and kinetics of reactive intermediates, Photochromic reactions and memory devices, Sensors, Switches and molecular machines, TiO<sub>2</sub> photocatalysis, Photosynthesis (plants), Intermediates in photoreactions, Identification and characterization through modern techniques, Flash photolysis, CIDNP, Photoacoustic, Stepscan IR.

**SECTION-C****6. Electrochemistry of Solutions: (15 Hrs)**

Ion-solvent interactions, the Born model, electrostatic potential at the surface of a charged sphere, Born expression for the free energy of ion-solvent interactions, structural treatment of ion-solvent interactions, ion-dipole moment, evaluation in the ion-dipole approach to heat of solvation, solvation number, static and dynamic pictures of ion-solvent interactions, hydration number, dielectric constant of water and ionic solutions, dielectric constant of liquids containing associated dipoles, ion – solvent nonelectrolyte interactions, change in solubility of non-electrolyte due to primary and secondary solvations.

**Course Outcomes:**

CO1	MCHE-2313.1	To impart advance knowledge of Principles and Concepts of  Laws of photochemistry
CO2	MCHE-2313.2	Understand reaction mechanism and kinetics of reaction mechanism and stability of Electronically Excited State
CO3	MCHE-2313.3	Understand the basic concept of Theory of Photoreactions
CO4	MCHE-2313.4	Provide an overview of field of Applications of Photochemistry and Photophysical Principles

**Books Recommended:**

1. Lakowicz, J. R., Principles of Fluorescence Spectroscopy, Springer, New York (2006), 3rd ed.

PCY--- P

2. Physical Chemistry, P.W. Atkins

**SUBJECT TITLE: Physical Chemistry Lab-II****SUBJECT CODE: MCHE-2314****SEMESTER: III****CONTACT HOURS/WEEK:**

Lecture (L)	Tutorial (T)	Practical (P)	Credit (C)
3	0	0	3

**Internal Assessment: 40****End Term Exam: 60****Duration of Exam: 3 Hrs**

**Course Objective:** To acquire knowledge of Chemical kinetics & chromatography techniques.

### 1. Chemical kinetics

(i) Reaction between Potassium bromate and Potassium Iodide : (a) To study the kinetics of reaction between Potassium bromate and Potassium Iodide catalyzed by  $H^+$  ions at room temperature. (b) To study the kinetics of reaction between Potassium bromate and Potassium Iodide catalyzed by  $H^+$  ions at least at three temperatures and hence to find out the activation energy of the reaction.

(ii) To study the reaction between  $H_2O_2$  and HI by clock method at least at three temperatures and hence to find out the activation energy of the reaction.

(iii) To study the kinetics of hydrolysis of tert butyl chloride by conductance measurements.

### 2. Phase Rule Three component system

(i) To study the limit of homogeneity of three components (i.e., benzene, acetic acid and water) system. (ii) To study the limit of homogeneity of three components (i.e., chloroform, acetic acid and water) system.

### 3. Thin Layer Chromatography

## Program Code: MCHE-401

(i) To separate and Identify the given mixtures of coloured compounds (azobenzene, hydroxyazobenzene, p-aminoazobenzene).

(ii) To separate and identify the given mixture of colourless compounds (Diphenylamine, Benzophenone, Naphthalene, and biphenyl).

(iii) To draw calibration curve for different amounts of Azobenzene after separating on TLC Plates, extracting with methanol and measuring with spectrophotometer and hence to find the amount of Azobenzene in its unknown sample.

#### 4. Cryoscopy

(i). To find the molar weight of the given solute in water by depression in freezing point method.

(ii). To find the values of van't Hoff factor and degree of dissociation of weak electrolytes by cryoscopic method.

(iii) To determine the degree of association of benzoic acid in benzene by cryoscopic method.

(iv) To determine the mean activity coefficients of strong electrolytes.

(v) Find the oscillator strength of the main band of diphenylamine in the ultraviolet region of the spectrum

#### Course Outcomes:

CO1	MCHE-2314.1	To impart advance knowledge of chromatography techniques
CO2	MCHE-2314.2	To acquire knowledge of Chemical kinetics
CO3	MCHE-2314.3	To understand Phase Rule Three component system
CO4	MCHE-2314.4	To separate and Identify the given mixtures of coloured compounds by thin Layer Chromatography

#### Recommended Books

1. Advanced Physical Chemistry Practical by J.B. Jadav.



Program Name: Masters in Chemistry

Program Code: MCHE-401

# **SEMESTER IV**

**SUBJECT TITLE: Bio-Inorganic Chemistry****SUBJECT CODE: MCHE-2401****SEMESTER: IV****CONTACT HOURS/WEEK:**

Lecture (L)	Tutorial (T)	Practical (P)	Credit (C)
3	0	0	3

**Internal Assessment: 40****End Term Exam: 60****Duration of Exam: 3 Hrs**

**Course Objective:** To impart advance knowledge of enzymes and metal ions in biological systems

### **Section-A**

#### **1. Inorganic Chemistry of Enzymes: (18 Hrs.)**

Introduction, energy sources for life, non-photosynthetic processes, metalloporphyrins, cytochromes, biochemistry of iron, iron storage and transport, ferritin transferring, bacterial iron transport, hemoglobin and myoglobin, nature of heme-dioxygen binding, model systems, cooperativity in hemoglobin, physiology of myoglobin and hemoglobin, structure and function of hemoglobin. Other iron-prophyrin biomolecules, structure and function of hemoglobin. Other iron-porphyrin biomolecules, peroxidases and catalases, cytochrome P450 enzymes, other natural oxygen carriers, hemerythrins, electron transfer, respiration and photosynthesis; ferridoxins, and subredonim carboxypeptidase, carbonic anhydrase, metallothioneins. Blue copper proteins, superoxide dismutase hemocyanines photosynthesis, chlorophyll and photosynetic reaction center.

### **Section-B**

#### **2. Metal Ions in Biological Systems: (18 Hrs)**

Metal complexes of polynucleotides, nucleosides and nucleic acids (DNA & RNA). Template temperature, stability of DNA. Role of metal ions in replication and transcription process of



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nucleic acids. Biochemistry of dioxygen, bioinorganic chips and biosensors. Biochemistry of calcium as hormonal messenger, muscle contraction blood clotting, neurotransmitter, calcification reclaiming of barren land. Metals in the regulation of biochemical events. Transport and storage of metal ions *in vivo*. Metal complexes as probes of structure and reactivity with metal substitution.

**Section-C**

**3. Inorganic Medicinal Chemistry: (9 Hrs)**

Fundamentals of Toxicity and Detoxification. Nuclear medicines.

**Enzymes:** Structure and function, inhibition and poisoning Vitamin B<sub>12</sub> and B<sub>12</sub> coenzymes metallothioneins, nitrogen fixation, in-vitro and in-vivo nitrogen fixation, bio-inorganic chemistry of Mo and W, nitrogenases: other elements V, Cr, Ni (essential and trace elements in biological systems).

**Course Outcomes:**

CO1	MCHE-2401.1	To impart advance knowledge of biochemical reaction in different biological systems with different techniques
CO2	MCHE-2401.2	Students will build a scientific temper and will be able to learn the necessary skills to succeed in biophysical chemistry area.
CO3	MCHE-2401.3	Provide an overview of field of biochemistry and natural product chemistry, their occurrence, structure, total synthesis, biosynthesis and properties.
CO4	MCHE-2401.4	Explain on mechanistic level, reactions and synthesis of important nitrogen/oxygen/Sulphur containing heterocycles; pyrroles, pyridines.

**Books Recommended:**

1. J. E. Huheey, E. A. Keiter and R.L. Keiter, Inorganic Chemistry Principles of Structure and Reactivity, 4th Edition, Haper Collins.
2. B. Douglas, D. McDaniel and J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edition, John Wiley and Sons.
3. F.A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry: A Comprehensive Text, 5th Edition, John Wiley.
4. Ch. Elschenbroich and A. Salzer, Organometallics. A Concise Introduction, Second Edition, VCH.
5. D.F. Shriver and P.W. Atkins, Inorganic Chemistry, 3rd Edition, Oxford University Press.

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6. J.A. Cowan, *Inorganic Biochemistry*, 2nd Edition, Wiley – VCH.
7. G. Wulfsberg, *Inorganic Chemistry*, University Science Books.
8. S.J. Lippard, & J. M. Berg *Principles of Bioinorganic Chemistry* Univ. Science Books (1994).
9. S. J. Lippard, *Progress in Inorganic Chemistry* Vols. 18 and 38, Wiley-Interscience

**SUBJECT TITLE: Biosynthesis of Natural Products**

**SUBJECT CODE: MCHE-2402**

**SEMESTER: IV**

**CONTACT HOURS/WEEK:**

Lecture (L)	Tutorial (T)	Practical (P)	Credit (C)
3	0	0	3

**Internal Assessment: 40**

**End Term Exam: 60**

**Duration of Exam: 3 Hrs**

**Course Objective:** To acquire knowledge of natural products and their metabolism

**Section-A**

**1. Introduction: (4 Hrs)**

Functions of metabolism. Primary and secondary metabolism. Biochemical reactions and organic reaction mechanisms. Principle Pathways and technique of elucidation metabolic sequences. The one carbon fragment.

**2. Primary Metabolism: (10 Hrs)**

General introduction to catabolic and anabolic pathways. Regulation of metabolic pathways. Structure and functions of ATP, free energy of hydrolysis of ATP. Photosynthesis. Carbohydrate metabolism-Glycolysis, Citric acid cycle, Glycogenesis Glycogenolysis and Glyconeogenesis, pentose phosphate Pathway. Electron Transport System and Oxidative Phosphorylation.

**Section-B**

**3.Secondary Metabolism: Metabolites derived from acetate (polyketide pathway): (6 Hrs)**

Biosynthesis of unsaturated and saturated fatty acids, prostaglandins, polyphenols *viz.* Orsellinic acid, 6-methylsalicylic acid, usnic acid, penicillic acid, patulin, citrinin, griseofluvin, alizarin, emodin, tetracyclines.

**Metabolites derived from mevalonic acid pathway (Terpenes): (10 Hrs.)**

Biosynthesis of mevalonic acid and the active isoprene units, monoterpenes *viz.* Citral, geraniol, pinene, camphor, terpineol, thujone, isobornylene, menthol, artemesia alcohol, santolina alcohol, Iridoids, *viz.* Loganin, iridomyrmecin, secolaganin, sweroside. Sesquiterpenes, *viz.* Humulene, -cedrene, -bisabolene, ovalicin, juvenile hormone, Diterpenes, *viz.* Phytol, Sclareol, abietic acid, taxinine. Triterpenes, squalene, lanosterol, cholesterol, cycloartenol, sitosterol, Vitamin D. Biological functions of steroids. Biosynthesis of carotenoids, *viz.* -carotene, - carotene, vitamin A.

**Section-C**

**Metabolite derived from shikimic acid pathway: (3 Hrs)**

Biosynthesis of shikimic acid, aromatic amino acids, cinnamic and benzoic acid, coumarines.

**The Alkaloids : (4Hrs)**

Biosynthesis of coacin, tropine, pseudopelletierine, coniine, nicotine, sparteine, ephedrine, morphine, quinine.

**4. Amino acids, Peptides and Proteins: (8Hrs)**

Introduction, amino acid classification and structure, chemical and enzymatic hydrolysis of proteins to peptides, amino acid sequencing. Secondary structure of proteins, forces responsible for holding secondary structures. - helix and -sheet. Tertiary structure of protein folding. Quaternary structure. Biosynthesis of amino acids.

**Course Outcomes:**

CO1	MCHE-2402.1	Understand the basic concept of organic chemistry.
CO2	MCHE-2402.2	To impart advance knowledge synthesis of organic compounds and organic reactions.

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CO3	MCHE-2402.3	Describe and demonstrate the importance of molecular rearrangements in organic compound synthesis and understand the basics of photochemistry and pericyclic reactions.
CO4	MCHE-2402.4	Describe the interaction of excited states with their surroundings and analyze photo-induced electron transfer/excitation energy transfer reaction.

**Books Recommended:**

1. Primary Metabolism: A Mechanistic Approach by J. Staunton, Oxford University Press, 1978.
2. Secondary Metabolism by J. Mann, Oxford University Press, Oxford, 1980.
3. Natural Product Chemistry - A mechanistic, Biosynthetic and Ecological Approach by Kurt B. G. Torssell, Swadish Pharmaceutical Society, 1997.
4. Principles of Biochemistry by A. L. Lehninger, CBS Publishers, New Delhi.
5. Fundamental of Biochemistry by D. Voet, J.G. Voet and C.W. Pratt, John Willey & Sons Inc., New York, 1999.

**SUBJECT TITLE: Bio-Physical Chemistry**

**SUBJECT CODE: MCHE-2403**

**SEMESTER: IV**

**CONTACT HOURS/WEEK:**

Lecture (L)	Tutorial (T)	Practical (P)	Credit (C)
3	0	0	3

**Internal Assessment: 40**

**End Term Exam: 60**

**Duration of Exam: 3 Hrs**

**Course Objective:** To impart advance knowledge of biochemical reaction in different biological systems with different techniques

**Section-A**

**1. Biological Cell and its Constituents: (5 Hrs)**

## Program Code: MCHE-401

Biological Cell, structure and functions of proteins, enzymes, DNA and RNA in living systems. Helix coil transition.

**2. Bioenergetics: (5 Hrs)**

Standard free energy change in biochemical reactions, exergonic, endergonic, Hydrolysis of ATP, synthesis of ATP from ADP, coupled reactions, degree of coupling.

**3. Statistical Mechanics in Biopolymers: (5 Hrs)**

Chain configuration of macromolecules, statistical distribution end to end dimensions, calculation of average dimensions for various chain structures. Polypeptide and protein structures, introduction to protein folding problem.

**4. Biopolymer Interactions: (5 Hrs)**

Forces involved in biopolymer interactions, Electrostatic charges and molecular expansion, hydrophobic forces, dispersion force interactions. Multiple equilibria and various types of binding processes in biological systems. Hydrogen ion titration curves.

**5. Thermodynamics of Biopolymer Solutions: (5 Hrs)**

Thermodynamics of biopolymer solutions, osmotic pressure, membrane equilibrium, muscular contraction and energy generation in mechanochemical system.

**Section-B****6. Cell Membrane and Transport of Ions: (5 Hrs)**

Structure and functions of cell membrane. Active transport across cell membrane, irreversible thermodynamics treatment of membrane transport.

**7. Structural Determination of Biological Macromolecules: (5 hrs)**

**Bio-polymers and their Molecular Weights:** Evaluation of size, shape, molecular weight and

extent of hydration of biopolymers by various experimental techniques.

**Viscosity:** Measurement, relation to geometry and correlation with hydrodynamic properties.

**Diffusion:** Fick's Law of diffusion, diffusion coefficient and its interpretation, frictional coefficient.

**Section-C**

**8. Techniques: (10Hrs)**

**Ultracentrifugation:** Svedberg equation, sedimentation equilibrium, density gradient sedimentation.

**Electrophoresis:** General principles, Double layer techniques, moving boundary electrophoresis,  
zonal electrophoresis, isoelectric focusing.

**Osmotic Pressure:** Second virial coefficient, Donnan effect, molecular mass and geometry from O.P. data.

**Optical Properties of Biomacromolecules:** Light Scattering, fundamental concepts, Rayleigh Scattering, Scattering by Larger particles.

**Methods for the Separation of Biomolecules:**

General principles, including Chromatography, Sedimentation, Moving Boundary Sedimentation, Zonal Sedimentation, Electrophoresis, Isoelectric focusing, Capillary electrophoresis, MALDI-TOF.

**Course Outcomes:**

CO1	MCHE-2403.1	Understand the basic concept of research and importance of seminars and research articles
CO2	MCHE-2403.2	To impart advance knowledge of chemistry based on research on chemistry
CO3	MCHE-2403.3	The practice of industrial visit to motivate students to take up their career in chemical industry and multinational companies based on research data.
CO4	MCHE-2403.4	Prepare the students for writing manuscripts based on the research output from their M.Sc. dissertation work.

**Books Recommended:**

1. Principles of Biochemistry, A.L. Lehninger, Worth Publishers.
2. Biochemistry, L. Stryer, W.H. Freeman.
3. Biochemistry, Voet and Voet, John Wiley.
4. Macromolecules: Structure and Function, F.Wold., Prentice Hall.
5. Text Book of Polymer Science, F.W. Billmeyer.
6. Physical Chemistry of Polymers, A. Tager.

**SUBJECT TITLE: Analytical Chemistry****SUBJECT CODE: MCHE-2404****SEMESTER: IV****CONTACT HOURS/WEEK:**

Lecture (L)	Tutorial (T)	Practical (P)	Credit (C)
3	0	0	3

**Internal Assessment: 40****End Term Exam: 60****Duration of Exam: 3 Hrs**

**Course Objective:** To impart advance knowledge of different analytical techniques for chemical analysis.

#### SECTION-A

##### 1. Introduction to analytical chemistry: (4 Hrs)

Methods of quantitative analysis, chemical analysis with its scale of operation, various steps in quantitative analysis.

##### 2. Sampling in analysis: (4 Hrs)

Theory of sampling importance of selecting a representative sample, criterion of a good sampling plan, Stratified sampling Vs. random sampling. Minimisation of variation in stratified sampling, sampling plan for solids, liquids and gases.

##### 3. Reliability of analytical data: (5 Hrs)

Errors in chemical analysis, classification of errors, Minimisation of errors, accuracy and precision. Improving accuracy of analysis, correlation and Regression, linear regression. Analysis of variance.

#### SECTION-B

##### 4. Polarography: (8 Hrs)

Principle, residual, Migration, diffusion currents, polarographic maximum, advantages and disadvantages of D.M.E. Reversible & irreversible processes, fundamental equation of polar

Program Code: MCHE-401

graphic wave. Derivation of Ilkovic equation & deviations, Quantitative technique & evaluation of quantitative results, Amperometric titrations & Biampometric titrations.

**5. Basic Principles of related technique of Polarography: (6 Hrs)**

Alternating current, Square Wave, pulse (normal and Differential) Tensometry, radio frequency and computer controlled polarograph.

**6. Chronoptentiometry: (2 Hrs)**

Theory, circuit and applications & comparison with polarography.

**SECTION-C**

**7. Thermo Analytical Methods: (8 Hrs)**

Thermogravimetric analysis, Introduction, Instrumentation, Factors affecting thermogravimetric results, applications of Thermogravimetry.

Differential Thermal analysis and differential scanning calorimetry on line analysis.

Thermometric titrations Introduction theory and applications.

**8. Spectrophotometry and Colorimetry: (8 Hrs)**

Theory of spectrophotometry and colorimetry, Beer's law, Deviation from Beer's law, absorptivity, Photometric accuracy. Spectrophotometric titrations and titration curves and applications to quantitative analysis.

Ion Exchange Resins : Different types of Ion exchangers and their synthesis. Ion exchange chromatography. Applications in analytical chemistry (a) Total cation Conc in tap water (b) Cu (II) from a brine solution U (VI) by liquid ion exchanger (d) use of mixed solvents.

**Course Outcomes:**

CO1	MCHE-2404.1	Understand the basic concept of research and importance of seminars and research articles
CO2	MCHE-2404.2	To impart advance knowledge of chemistry based on research on chemistry
CO3	MCHE-2404.3	The practice of industrial visit to motivate students to take up their career in chemical industry and multinational companies based on research data.
CO4	MCHE-2404.4	Prepare the students for writing manuscripts based on the research output from their M.Sc. dissertation work.

**Books Recommended:**



## Program Code: MCHE-401

1. Chemical analysis by Lattinen Harris.
2. Modern Polarographic methods in Analytical Chemistry A. M. Bend.
3. Instrumental methods of analysis Willard, Merrit and Dean.
4. Vogel's Quantitative Inorganic analysis.
5. Vogel's Quantitative Chemical analysis.
6. Basic concepts of analytical Chemistry BY S. M. Khopkar

**SUBJECT TITLE: Physical Chemistry Lab-III****SUBJECT CODE: MCHE-2405****SEMESTER: IV****CONTACT HOURS/WEEK:**

Lecture (L)	Tutorial (T)	Practical (P)	Credit (C)
0	0	6	3

**Internal Assessment: 40****End Term Exam: 60****Duration of Exam: 3 Hrs****(i) Conductance Measurements**

1. Acid-base Titrations (a) Strong acid vs strong base. (b) Weak acid vs strong base. (c) Strong acid vs weak base. (d) Mixture of strong acid and weak acid vs strong base. (e) Mixture of strong acid, Weak acid and CuSO<sub>4</sub> vs strong base.
2. To determine the cell constant of the given conductivity cell.
3. Determination of the solubility of sparingly soluble salts.
4. Verification of Debye-Huckel-Onsagar equation.
5. Verification of Ostwald dilution law.
6. Transport number measurements by Hittorf's method.
7. Precipitation titrations.
8. Complexometric titrations.
9. Determination of the degree of hydrolysis of the salts.

**(ii) E.M.F. Measurements (Potentiometry)**

1. Volumetric analysis. (a) Acid-base titrations. (b) Precipitation titrations. (c) Redox titrations.
2. Construction and determination of emf of the following cells : (a) Pt./Hg, Hg<sub>2</sub>Cl<sub>2</sub> , KCl (saturated) / Ag<sup>+</sup> (0.1N)/ Ag (b) Pt./Hg Hg<sub>2</sub>Cl<sub>2</sub> , KCl (0.1) / Ag<sup>+</sup> (0.1 N) / Ag (c) Ag / Ag<sup>+</sup> (0.01N)/Ag<sup>+</sup> (0.1N) Ag (d) Ag / Ag<sup>+</sup> (0.01N) / KCl (0.01N) AgCl / Ag
3. Determination of the solubility of the sparingly soluble salts.

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4. Determination of the mean activity coefficients.  
 5. To determine the various thermodynamic functions for the following reaction :  $Zn + Cu^{2+} \rightleftharpoons Zn^{2+} + Cu$   
 6. To determine the equilibrium constant for the complex,  $[Ag(NH_3)_4]^+$  formation.

**(iii) Flame Photometry**

To determine the concentration of the ions like  $Na^+$ ,  $K^+$ ,  $Ca^{2+}$  in the given solution.

**Course Outcomes:**

CO1	MCHE-2405.1	Understand the basic concept of research and importance of seminars and research articles
CO2	MCHE-2405.2	To impart advance knowledge of chemistry based on research on chemistry
CO3	MCHE-2405.3	The practice of industrial visit to motivate students to take up their career in chemical industry and multinational companies based on research data.
CO4	MCHE-2405.4	Prepare the students for writing manuscripts based on the research output from their M.Sc. dissertation work.

**Books Recommended:**

Advanced Physical chemistry Practical By J.B. Yadav.

**Optional Subjects (Inorganic Chemistry)**

**SUBJECT TITLE: Inorganic Chemistry - IV**

**SUBJECT CODE: MCHE-2406**

**SEMESTER: IV**

**CONTACT HOURS/WEEK:**

Lecture (L)	Tutorial (T)	Practical (P)	Credit (C)
3	0	0	3

**Internal Assessment: 40**

**End Term Exam: 60**

**Duration of Exam: 3 Hrs**

**Course Objective:** To impart advance knowledge of different inorganic compounds and their applications in biological systems.

**1. Inorganic chains, rings and cages (15 Hrs.):**

**Chains:** Catenation, heterocatenation, isopolyanions and heteropolyanions.

Program Code: MCHE-401

**Rings:** Borazines, phosphazenes, other heterocyclic inorganic ring systems, homocyclic inorganic systems.

**Cages:** Cage compounds having phosphours, oxygen, nitrogen and sulphur: boron cage compounds, Boranes, carboranes and metallocene carboranes.

**2. Transition metal cluster compounds (15 Hrs.):**

Introduction, metal carbonyl clusters; Low Nuclearity (M3 M4) clusters: isoelectronic and isolobal relationships high nuclearity carbonyl clusters; hetero atoms in metal atom clusters, electron counting schemes for HNCC: HNCC of Fe, Ru, Os, Co, Rh, Ir, Ni, Pd, Pt.

Lower halide and chalcogenide clusters, octahedral metal halide, chalcogenide clusters, triangular clusters, solid state extended arrays.

Compounds with M-M multiple bonds; I) Major structural types; quadrupole bonds, other bond orders in the tetragonal context, relation of clusters to multiple bonds, one dimensional solids.

**3. Inorganic Chemistry in Biological Systems (15 Hrs.):**

Porphyrin rings, metalloporphyrins, photosynthesis and respiration, chlorophyll, structure, function and synthetic model Cytochromes; structure and function, CN and CO poisoning, Farredoxins and rubberdoxins, bioredox agents and mechanism, Hemoglobin and myoglobin, structure and mechanism of function, Cooperatively, Enzymes, Vitamin B<sub>12</sub>, B<sub>12</sub> Coenzymes; structures and function, synthetic model of enzyme action, inhibition on poisoning by ligands and metal ions xanthine oxidase, N<sub>2</sub> fixation.

**Course Outcomes:**

CO1	MCHE-2406.1	To impart advance knowledge of different inorganic compounds and their applications in biological systems.
CO2	MCHE-2406.2	Students will build a scientific temper and will be able to learn the necessary skills to succeed in biophysical chemistry area.
CO3	MCHE-2406.3	To impart advance knowledge of enzymes and metal ions in biological systems
CO4	MCHE-2406.4	To impart the knowledge of biochemistry in daily life

**Books Recommended:**

**Program Code: MCHE-401**

1. J.E.Huheey, Inorganic Chemistry, 3rd Edition, London, 1983.
2. F.A. Cotton, I.G. Wilkinson, Advanced Inorganic Chemistry, 5th Edition, New York, 1988.
3. D.F. Shriver, P.W. Atkins and C.H. Langford, Inorganic Chem., ELMS, Oxford, 1990

**SUBJECT TITLE: Photo Inorganic Chemistry****SUBJECT CODE: MCHE-2407****SEMESTER: IV****CONTACT HOURS/WEEK:**

Lecture (L)	Tutorial (T)	Practical (P)	Credit (C)
3	0	0	3

**Internal Assessment: 40****End Term Exam: 60****Duration of Exam: 3 Hrs**

**Course Objective:** To impart advance knowledge of photochemistry and photochemical process

#### **Section-A**

##### **1. Basics of photochemistry: (8 hrs)**

Absorption, excitation, photochemical laws, quantum yield, electronically excited states- life times-measurements of the times. Flash photolysis, stopped flow techniques. Energy dissipation by radiative and non-radiative processes, absorption spectra, Franck-Condon principle, photochemical stages- primary and secondary processes

##### **2. Properties of excited states: (5 hrs)**

Structure, dipole moment, acid-base strengths, reactivity. Photochemical calculation of rates of radiative processes. Bimolecular deactivation - quenching kinetics III

#### **Section-B**

##### **3. Excited states of metal complexes: (8 hrs)**

Excited states of metal complexes: comparison with organic compounds, electronically excited states of metal complexes, charge-transfer spectra, charge transfer excitations, methods for obtaining charge-transfer spectra.

##### **4. Ligand field photochemistry: (8 hrs)**

Program Code: MCHE-401

Photosubstitution, photooxidation and photoreduction, lability and selectivity, zero vibrational levels of ground state and excited state, energy content of excited state, zero-zero spectroscopic energy, development of the equations for redox potentials of the excited states.

**Section-C**

**5. Reactions by excited metal complexes: (10 hrs)**

Energy transfer under conditions of weak interaction and strong interaction-exciple formation; conditions of the excited states to be useful as redox reactants, excited electron transfer, metal complexes as attractive candidates (2,2'-bipyridine and 1,10-phenanthroline complexes), illustration of reducing and oxidising character of Ruthenium<sup>2+</sup>(bipyridal complex, comparison with Fe(bipy)<sub>3</sub>); role of spin-orbit coupling-life time of these complexes. Application of redox processes of electronically excited states for catalytic purposes, transformation of low energy reactants into high energy products, chemical energy into light

**6. Metal complex sensitizer: (6hrs)**

Metal complex sensitizer, electron relay, metal colloid systems, semiconductor supported metal or oxide systems, water photolysis, nitrogen fixation and carbon dioxide reduction

**Course Outcomes:**

CO1	MCHE-2407.1	To impart advance knowledge of photochemistry
CO2	MCHE-2407.2	To understand Energy transfer under conditions of weak interaction and strong interaction-exciple formation
CO3	MCHE-2407.3	Provide an overview of field of biochemistry and natural product chemistry, their occurrence, structure, total synthesis, biosynthesis and properties.
CO4	MCHE-2407.4	Explain on mechanistic level, reactions and importance of Metal complex sensitizer

**Books Recommended:**

1. Concepts of Inorganic Photochemistry, A.W. Adamson and P.O. Fleischauer, Wiley.
2. Inorganic Photochemistry, J. Chern. Educ., vol. 60, no. 10, 1983.
3. Progress in Inorganic Chemistry, vol. 30, ed. S.J. Lippard, Wiley.
4. Coordination Chern. Revs., 1981, vol. 39, 121, 131; 1975, 15, 321; 1990,97,313.
5. Photochemistry of Coordination Compounds, V. Balzari and V. Carassiti, Academic Press.

6. Elements of Inorganic Photochemistry, G. J. Ferraudi, Wiley

**SUBJECT TITLE: Inorganic Chemistry Lab-III**

**SUBJECT CODE: MCHE-2408**

**SEMESTER: IV**

**CONTACT HOURS/WEEK:**

Lecture (L)	Tutorial (T)	Practical (P)	Credit (C)
0	0	6	3

**Internal Assessment: 40**

**End Term Exam: 60**

**Duration of Exam: 3 Hrs**

**Course Objective:** To impart knowledge of synthesis of Inorganic compounds.

### EXPERIMENTS

**1** Preparation of mercury tetrakisothiocyanatocobalt(II). Determination of its magnetic moment and interpretation of its IR spectrum.

**2** Preparation of nitro-and nitrito-pentaamminecobalt(II) chlorides from chloropenta amine cobalt(III) chloride. Recording and interpreting their electronic and IR spectra.

**3** Heating the nitro and nitrito isomers at serial 2 to 15°C in an oven for 3 h and recording the infrared spectra again and compare them with the spectra recorded before the isomers were heated.

Program Code: MCHE-401

**4** Preparation and resolution of tris(ethylenediamine)cobalt(II) ion. Measurement of optical rotation of these resolved complexes.

**5** Preparation of diaquotetraacetatedicopper(II). Determination of its magnetic susceptibility and interpretation of E.P.R., electronic absorption and IR spectra.

**6** Preparation of bis(2,4-pentanedione)vanadium(IV) acetate and its piperidine or pyridine complex. Study of both the complexes with the help of infrared, UV-vis spectroscopy and magnetic susceptibility.

**7** Preparation of hexaamminenickel(II) chloride and tris(ethylenediamine)nickel(II) chloride. Interpretation of their electronic absorption spectral data and calculation of  $\beta$  and  $10Dq$  values. Measurement of magnetic susceptibility, calculation and interpretation of the values.

**8** Preparation of lead tetraacetate.

**9** Preparation of potassium trioxalatoaluminate(III) trihydrate. Its TGA and DTA studies and its interpretation of its i.r. data.

**10** Preparation of disulphur dichloride

**11** Preparation of sodium tetrathionate, potassium dithionate, and interpretation of their IR spectra.

**12** Preparation of cis-and trans-potassium dioxalato diaquochromate (III). Interpretation of their i.r., and electronic absorption spectral data. Calculation of  $\beta$  and  $10 Dq$  values.

**Course Outcomes:**

CO1	MCHE-2408.1	To impart advance knowledge of synthesis of Inorganic compounds
CO2	MCHE-2408.2	Students will build a scientific temper and will be able to learn the necessary skills to succeed in inorganic chemistry
CO3	MCHE-2408.3	To detect and explain magnetic and spectroscopy properties of complexes
CO4	MCHE-2408.4	Explanation and understanding of TGA and DTA of complexes

**Books Recommended:**

**1** G. Marr and B.W. Rockett: Practical Inorganic Chemistry, Van Nostrand Reinhold Company

**2** W.L. Jolly, The Synthesis and Characterization of Inorganic Compounds. Prentice



**Optional Subjects (Organic Chemistry)****SUBJECT TITLE: Modern Synthetic Reactions and Rearrangements****SUBJECT CODE: MCHE-2409****SEMESTER: IV****CONTACT HOURS/WEEK:**

Lecture (L)	Tutorial (T)	Practical (P)	Credit (C)
3	0	0	3

**Internal Assessment: 40****End Term Exam: 60****Duration of Exam: 3 Hrs**

**Course Objective:** To impart advance knowledge of mechanism of organic complexes and their application

### Section-A

#### 1. Fictionalization of Non Activated Carbon (13 Hrs)

Barton's reaction and related process mechanism, stereochemistry of transition state, photolysis of organic nitrites, N-Nitrosoamides, hypohalites. Reaction of monohydric alcohols with lead tetraacetate, olefinic alcohols from hydroperoxides, cyclobutanols from photolysis of ketones, applications to steroid nucleus.

Hoffman Ley Freytag Reaction using N-chloramine derivatives, mechanistic approach and application.

Newer Chemical Techniques: Brief concept of crown ethers, phase transfer reagent, application in synthesis.

Use of compounds of Thallium (III), Palladium and Ruthenium oxide in organic synthesis.

### Section-B

#### 2. Organosilicon: (7 Hrs)

New application of organosilicon compounds in synthesis, protection of functional group, trimethylsilylcyanide, elimination from  $\beta$ -hydroxy-silane, the Peterson reaction and related process; Annelation; alkenylsilanes and  $\alpha$ ,  $\beta$ -epoxysilanes, stabilisation of carbonium ions by  $\beta$ -silyl groups.

#### 3. Allylic alkylation of alkenes: (6 Hrs)

The dihydro 1,3-oxazine synthesis of aldehyde and ketones, coupling of organonickel and organocopper complexes. Reaction of lithium organocuprates, synthetic application of carbenes and carbenoids. Some photocyclisation reactions, acyclic conjugated trienes, stilbene, Anil, alkaloids and related processes.

### Section-C

#### 4. Rearrangements in Small Ring Compounds (10 Hrs)

Program Code: MCHE-401

Introduction : Thermal rearrangements, Cyclopropane derivatives, Acid catalyzed rearrangement involving carbonium ions, Base catalysed rearrangement, involving carbanions, Rearrangements involving free radicals and carbene intermediate.

**5. Thermal rearrangements :** Cyclobutane derivatives, Acid catalysed rearrangement involving carbonium ion, base catalysed rearrangement involving carbanions, Rearrangements involving free radical and carbene intermediate.

**6. Rearrangement in Steroids (9 Hrs)**

Angular group migration, Rearrangement in C<sup>13</sup>-CH<sub>3</sub>, C<sup>9</sup>, C<sup>11</sup>, C<sup>19</sup> methyl groups. Dienone phenol rearrangement. Anthrasteroid Rearrangement. Retro aldol phenomenon. steroid transformation. Ring expansion and contraction in A, B, C, D Rings. Acyloin Rearrangement in D-homoannulation, Acyl group migration, Allylic transposition, Redistribution Reactions.

**Course Outcomes:**

CO1	MCHE-2409.1	To impart advance knowledge of reaction in different
CO2	MCHE-2409.2	Students will build a scientific skills to learn organosilicon and alkylation.
CO3	MCHE-2409.3	Rearrangments in Steroids
CO4	MCHE-2409.4	Rearrangments in Steroids

**Books Recommended:**

1. K. W. Bentley : Elucidation of Organic Structure by Physical Method, Part-I, II.
2. P. S. Kalsi : Chemistry of Natural Products.
3. P. de-Mayo : Molecular Rearrangement, Vol. I & II.
4. H. O. House : Modern Synthetic Reaction.
5. W. Carruther : Some Modern Methods of Organic Synthesis.

**SUBJECT TITLE: Heterocyclic Chemistry**

**SUBJECT CODE: MCHE-2410**

**SEMESTER: IV****CONTACT HOURS/WEEK:**

Lecture (L)	Tutorial (T)	Practical (P)	Credit (C)
3	0	0	3

**Internal Assessment: 40****End Term Exam: 60****Duration of Exam: 3 Hrs**

**Course Objective:** To introduce synthesis and reactivity of aliphatic and aromatic and heterocyclic compounds and molecular rearrangements in some heterocyclic compounds

#### **Section-A**

##### **1. Three membered ring with one heteroatom : (7 Hrs)**

Oxirane, Aziridine, Thirane : Introduction, synthetic methods, Direct insertion of heteroatom into carbon-carbon-double bond, methylene insertion reaction, cyclisation method, condensation reaction, Nucleophilic and Electrophilic ring opening. Reaction involving extrusion of the heteroatoms.

##### **2. Four membered Heterocyclics with one Heteroatom : (8 Hrs)**

Oxetane, Oxetene, thitenes, thitanes, Azetidines : Introduction, Synthetic method, Cyclisation reaction, Direct combination method, Reaction electrophilic, Nucleophilic ring opening and General chemical reactions.

#### **Section-B**

##### **3. Five membered Heterocyclics with two heteroatoms : (10 Hrs)**

Pyrazole and Imidazoles : Introduction, Physical properties, Structure, Synthetic method, Electrophilic and Nucleophilic reactions.

**4. Isoxazole and Oxazole :** Introduction, Physical and chemical properties of isoxazole and oxazoles and their derivatives.

Isothiazole and Thiazoles : Physical and chemical properties, synthetic reactions.

#### **Section-C**

##### **5. Six membered Heterocyclic with two heteroatoms. (20 Hrs)**

Introduction: Pyridazine, Pyrimidine, Pyrazine. Synthetic approaches. Chemical reactions; Electrophilic substitution, Nucleophilic substitution, Side chain reactivity.

Oxazines: Classification, nomenclature structure, Synthetic approaches and chemical reactions.

### 6. Molecular Rearrangement in some Heterocyclic compounds

#### I. Ring Contraction:

- (a) Pyridine and Quinoline derivatives to pyrrole & indole.
- (b) Benzodiazepirtes to Quinoxalenes and Benzimidazole derivatives.
- (c) Quinoxaline to Benzimidazoles.
- (d) Dihydro flavonols to Benzyl and Benzylidene Coumaranone.
- (e) Dihydrofurans to cyclopropyl ketone.

#### II. Ring Expansion :

- (a) Pyrrole to Pyridines.
- (b) Benzylidene Coumaranones to flavonones and flavonols.
- (c) Tetrahydro furfuryl alcohol to Dihdropyran.

#### III. 1, 2 Rearrangements in Heterocyclic system.

- (a) 1,2 - Rearrangement in catechin derivatives.
- (b) 1,2 - Rearrangement of indole derivatives.
- (c) 1,2 - Rearrangement during Clemmenson's Reduction.

#### Course Outcomes:

CO1	MCHE-2410.1	To introduce synthesis and reactivity of aliphatic and aromatic and heterocyclic compounds
CO2	MCHE-2410.2	molecular rearrangements in some heterocyclic compounds
CO3	MCHE-2410.3	Explain on mechanistic level, reactions and synthesis of important different member ring compounds
CO4	MCHE-2410.4	Explain on mechanistic level, reactions and synthesis of important nitrogen/oxygen/Sulphur containing heterocycles; pyrroles, pyridines.

#### Books Recommended:

1. R. M. Acheson: Chemistry of Heterocyclics.
2. A. R. Katrizky: Handbook of Heterocyclics.
3. Lee A. Paquette: Principles of Modern Heterocyclic Chemistry.
4. P-de-Mayo: Molecular Rearrangement, Vol.1.

**SUBJECT TITLE: Organic Chemistry Lab-III****SUBJECT CODE: MCHE-2411****SEMESTER: IV****CONTACT HOURS/WEEK:**

Lecture (L)	Tutorial (T)	Practical (P)	Credit (C)
0	0	6	3

**Internal Assessment: 40****End Term Exam: 60****Duration of Exam: 3 Hrs****Course Objective: To impart knowledge of advance organic synthesis****EXPERIMENTS**

**1** Synthesize (a) 2,4-dinitro-1-chlorobenzene from chlorobenzene, (b) mixture of *o*- and *p*-nitrophenols from phenol and (c) *p*-nitroacetanilide from acetanilide and make comparison of the reactivity of various substrates and reaction conditions used for performing nitration in each experiment.

**2** Synthesis of 2-chloro-4-bromo-6-iodoaniline from aniline.

**3** Synthesis of benzalacetophenone by condensation of benzaldehyde with acetophenone and study its bromination and subsequent debromination.

**4** The epoxidation of benzalacetophenone to its epoxide and study its reactivity towards hydroxyl ion.

**5** Michael addition of aniline to benzalacetophenone.

**6** Conversion of benzalacetophenone to its oxime and its transformation to amide and oxazole derivatives.

**7** Synthesis of anthranilic acid from phthalimide.

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8 Synthesis of p-aminobenzenesulfonamide.

9 Synthesis of Methyl n-pentyl ketone from ethyl acetoacetate.

10 Synthesis of triphenylcarbinol from bromobenzene.

**Course Outcomes:**

CO1	MCHE-2411.1	To impart knowledge of advance organic synthesis
CO2	MCHE-2411.2	Students will build a scientific temper and will be able to learn the necessary skills to succeed in synthesis of organic compounds.
CO3	MCHE-2411.3	The epoxidation and Michael addition reactions mechanism
CO4	MCHE-2411.4	Explain on mechanistic level, reactions and synthesis of important compounds by nitration method

**Books Recommended:**

1. An Introduction to Modern Experimental Organic Chemistry, R.M. Roberts, Gilbert, L.B. Rodewald and A.S. Wingrove. Holt, Ranehart and Winston Inc., J.C New York. 1969.
2. Vogel's Text Book of Practical Organic Chemistry, 5th Edition.
3. Laboratory Experiments in Organic Chemistry, R. Adams, J.R. Johnson and C.F. Wilcox, The Macmilan Limited, London, 1970

**Optional Subjects (Physical Chemistry)****SUBJECT TITLE: Biofuels****SUBJECT CODE: MCHE-2412****SEMESTER: IV****CONTACT HOURS/WEEK:**

Lecture (L)	Tutorial (T)	Practical (P)	Credit (C)
3	0	0	3

**Internal Assessment: 40****End Term Exam: 60****Duration of Exam: 3 Hrs**

**Course Objective:** To acquire knowledge of different methods of biofuel production, application, and their advantages.

**Section A****1. Introduction: (15 Hrs)**

Drivers for alternative fuels, security, cost and environmental considerations, carbon sequestration and the impact of biofuels, review of current processes for biofuel production from biomass. Economic Models: Costing of current and future processes for biofuel production from biomass, biomass availability, models of biomass concentration and utilization.

**Section B****2. Feedstock Chemistry: (15 Hrs)**

Chemistry of triglycerides and carbohydrates, Improving biomass yield and properties for easier processing and conversion, Pretreatment of biomass, Enzymatic hydrolysis, Processes and alternatives, Enzymes immobilization techniques.

**Section C****3. Fermentation: (15 Hrs)**

Processes and alternatives, Aqueous processing of sugars. Bio-Diesel and other alternative liquid fuels, Policy of biofuels, Biofuels around the world: Brazil, India and China. Course



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outcomes: The students will acquire the knowledge of biofuel production technologies, and their applications.

**Course Outcomes:**

CO1	MCHE-2412.1	This course will impart the understanding of alternative fuels and biofuels to students
CO2	MCHE-2412.2	Different processes and techniques related to conversion and storage energy.
CO3	MCHE-2412.3	Fundamental understanding of the Chemical, Electrochemical and Photochemical processes in Energy generation, storage and Utilization
CO4	MCHE-2412.4	Develop industry related skills and knowledge of industrial processes related to bioenergy

**Books Recommended:**

1. Bhojvaid, P.K., Biofuels: Towards a greener and secure energy future, TERI Press (2006).
2. Adholeya, A., and Kumar P., Dadhich Production and Technology of Bio-diesel: Seeding a change, TERI press (2008).
3. Scragg, A. H., Biofuels: Production, Application and Development, CABI (2009).
4. Olsson, L., Biofuels, Springer, (2007).
5. Furfari, A., Biofuels: Illusion Or Reality? : the European Experience, Editions TECHNIP (2008)

**SUBJECT TITLE: Surface Chemistry****SUBJECT CODE: MCHE-2413****SEMESTER: IV****CONTACT HOURS/WEEK:**

Lecture (L)	Tutorial (T)	Practical (P)	Credit (C)
3	0	0	3

**Internal Assessment: 40****End Term Exam: 60****Duration of Exam: 3 Hrs****Course Objective:** to impart knowledge of surface reactions, adsorption and catalysis**Section A****1. Adsorption: (9 Hrs)**

Adsorption, Adsorption of gases, influence of temperature and pressure, nature of adsorption and adsorbed gases, unimolecular layers, types of adsorption, Langmuir adsorption isotherm and BET adsorption equation, Freundlich and tempkin equation and their derivation, estimation of surface area of adsorption, Gibbs adsorption equation and its verification.

**2. Kinetics of Heterogeneous reaction at solid surface: (8 Hrs)**

Gas reaction on solids, single reacting gas, retardation of reaction products, two reacting gases, retardation by reactants and products, adsorption and desorption as rate determining, absolute rate theory of heterogeneous reactions.

**Section B****3. Catalysis: (8 Hrs)**

Catalyst and criteria of catalysis and initiation of a reaction. Catalytic activity and its determination, salt effects. Spectroscopic methods like PES, AES, LEED to determine surface structure. Important applications of surface chemistry, surfactant, wetting, micelles, detergency, surface tension, inter facial tension

**4. Surface phenomenon: (9 Hrs)**

Surface phenomenon, capillary action, pressure difference across surface (Lapace equation), Vapour pressure of droplets (Kelvin Equation). Heterogeneous catalysis, surface

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catalyzed unimolecular and bi molecular reactions, retarded surface reactions, temporary and permanent poisons, activation energy for surface reactions

**Section C****5. Physical Properties & Molecular Structure: (5 Hrs)**

Molar refraction, polarizability of molecules, dipole moment and its determination, dipole moment and structure of molecules.

**6. Colloidal State: (10 Hrs)**

Classification of colloids, charge and stability of colloidal dispersions, Hardy-Schulze Law, gold number, electrical properties of colloids, electrical double layer and its structure, Stern's theory of double layer, zeta-potential, electrophoresis and electroosmosis, emulsions and their classification, emulsifiers, gels and their classification, thixotropy. Association colloids; miceller formation, cmc, soap action. Application of colloids.

**Course Outcomes:**

CO1	MCHE-2413.1	To impart knowledge of surface reactions, adsorption and catalysis.
CO2	MCHE-2413.2	To understand the Kinetics of Heterogeneous reaction at solid surface
CO3	MCHE-2413.3	Provide an overview of field of Classification of colloids
CO4	MCHE-2413.4	Explain on mechanistic level, reactions and applications of molecular structure

**Books Recommended**

1. Principles of physical chemistry, S.H. Maron & C.F. Prutton.
2. Physical Chemistry, K.J. Laidler.
3. Physical Chemistry, P.W. Atkins.
4. Physical Chemistry of Polymers, A. Tager.
5. Text book of Polymers science, F.W. Billmeyer.
6. Heterogenous Catalysis, S.J. Thomson & G Webb.
7. Kinetics and Mechanism, A.A. Frost & R.G. Pearson.

**SUBJECT TITLE: Physical Chemistry Lab-IV****SUBJECT CODE: MCHE-2414****SEMESTER: IV****CONTACT HOURS/WEEK:**

Lecture (L)	Tutorial (T)	Practical (P)	Credit (C)
0	0	6	3

**Internal Assessment: 40****End Term Exam: 60****Duration of Exam: 3 Hrs**

**Course Objective:** To impart knowledge of Photochemistry & Phase equilibrium experiments.

### 1. PHOTOCHEMISTRY

(I) Intensity of the lamp/Quantum yield of the Reaction.

(a) To draw calibration curve for various concentrations of Ferrous sulphate/1,10-phenanthroline complex and hence to find the coefficient of its molar absorptivity.

(b) To find out the intensity of the lamp (visible light) by ferrioxalate actinometer

. (II) Methylene blue Sensitized photooxidation of Diphenylamine

(a) To study the rate of formation of the product in the above photochemical reaction with increasing quanta of light absorbed and to find the quantum yield of this reaction.

(b) To study the effect of following parameters on the above reaction

(1) Effect of dielectric constant of the medium.

(2) Effect of methylene blue concentration.

(3) Effect of diphenylamine concentrations.

(4) Effect of oxygen concentration.

### 2. TWO COMPONENT SYSTEMS

(a) To determine the critical solution temperature (CST) and critical solution concentration (CSC) for phenol/water system. .

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(b) To find the Eutectic point for two component systems, i.e., Naphthalene/Benzoic acid and benzoic acid/ Cinnamic acid systems.

**3. PARTIAL MOLAL VOLUMES**

To find the partial molal volumes for urea, sodium chloride and ethanol in aqueous solutions

**4. LEAST SQUARE PLOT**

To calculate the slope and intercept for a data of straight lines by least square method and to draw the line.

**5. MICELLES FORMATION**

(a) To determine the critical micelle conc. of sodium dodecyl sulphate from a study of the conductivity of aqueous solutions.

(b) To determine critical conc. for the formation of micelles from the spectral behaviour of a dye.

**Course Outcomes:**

CO1	MCHE-2414.1	To impart advance knowledge of micelles formation
CO2	MCHE-2414.2	Photochemistry reactions mechanism, Intensity of the lamp/Quantum yield of the Reaction
CO3	MCHE-2414.3	Understanding to determine the critical solution temperature (CST) and critical solution concentration
CO4	MCHE-2414.4	Understanding of partial molal volumes for some compounds

**Books Recommended:**

1. Findlay's Practical Physical Chemistry.
2. Advanced Practical Physical Chemistry by J.B. Yadav.



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