CRITERIA 1.1.2

The Programmes offered by the institution focus on employability/entrepreneurship/ skill development and their course syllabi are QM adequately revised to incorporate contemporary requirements.

Programme-

M.SC CHEMISTRY

Color Coding: -

1) **EMPLOYABILITY**

2) **ENTREPRENEURSHIP**

3) **SKILL DEVELOPMENT**

COURSE CURRICULUM
FOR
MASTER COURSES UNDER CHOICE BASED CREDIT SYSTEM

M.Sc. (CHEMISTRY)

DEPARTMENT OF CHEMISTRY

NETAJI SUBHAS UNIVERSITY, JAMSHEDPUR

With effective from academic session 2018

M. K. Mishra
Head
Department of Chemistry
Netaji Subhas University

NETAJI SUBHAS UNIVERSITY Jamshedpur 1

Dean Academics
Netaji Subhas University
Jamshedpur, Jharkhand

COURSE HAVING FOCUS ON SKILL DEVELOPMENT (SD), EMPLOYABILITY (EM), ENTREPRENEURSHIP (EN) IN M.SC. CHEMISTRY

Course Code	Name of Course	SD	EM	EN
MSCCHE -101	INORGANIC CHEMISTRY-1			✓
MSCCHE -102	ORGANIC CHEMISTRY -1			✓
MSCCHE -103	PHYSICAL CHEMISTRY -1			✓
MSCCHE -PR - 01	PRACTICAL-1			✓
MSCCHE -201	ANALYTICAL CHEMISTRY	✓	✓	✓
MSCCHE -202	GROUP THEORY & SPECTROSCOPY	✓	✓	✓
MSCCHE-203	PHYSICAL CHEMISTRY -2			✓
MSCCHE -PR - 02	PRACTICAL-2			✓
MSCCHE -301	APPLICATIONS OF SPECTROSCOPY	✓	✓	✓
MSCCHE -302	ENVIRONMENTAL CHEMISTRY	✓	✓	✓
MSCCHE-303	BIO-CHEMISTRY	✓	✓	✓
MSCCHE -PR - 03	PRACTICAL-3			✓
Group A				
MSCCHE -401A	PHYSICAL CHEMISTRY-III			✓
MSCCHE -402A	PHYSICAL CHEMISTRY-IV			✓
MSCCHE-403A	PROJECT WORK	✓	✓	✓
MSCCHE -PR-04A	PRACTICAL-4A	✓		✓
Group B				
MSCCHE -401B	INORGANIC CHEMISTRY-II			✓
MSCCHE -402B	INORGANIC CHEMISTRY-III	✓	✓	✓
MSCCHE-403B	PROJECT WORK	✓		✓
MSCCHE -PR-04B	PRACTICAL-4B			✓
Group C				✓
MSCCHE -401C	ORGANIC CHEMISTRY-II			✓
MSCCHE -402C	ORGANIC CHEMISTRY-III	✓	✓	✓
MSCCHE-403C	PROJECT WORK	✓		✓
MSCCHE -PR-04C	PRACTICAL-4C			

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NETAJI SUBHAS UNIVERSITY, JAMSHEDPUR

DEPARTMENT OF CHEMISTRY
PROGRAMME NAME: M.Sc. CHEMISTRY
CO, PO & PSO

VISION: The vision of the Department of Chemistry is to excel our status as an outstanding teaching and research institution.

MISSION:The mission of the Department of Chemistry is to provide high valued academic environment and to perform cutting edge research in versatile arenas of chemical sciences. To bring up advanced research programs those enhance knowledge through discovery and development.

To contribute actively the scientific community, and to engage itself with critical global needs for welfare of humanity. The department of chemistry is devoted to the development of students.

NETAJI SUBHAS UNIVERSITY Jamshedpur

Department of Chemistry	After successful completion of two year master program in Chemistry a student should be capable to;
Programme Outcomes	PO-1 (Scientific knowledge): Apply the knowledge of chemical science to find solutions to various academic and research problems. PO-2 (Problem analysis): Identify a research problem, review research literature, and design innovative solutions for scientific problems. PO-3 (Skill enhancement): Recognize and practice the required skillsets to enhance them for future employability. PO-4 (Modern tool usage): Adopt appropriate modern techniques, resources, and tools to execute the experiments and analyze and interpret the data. PO-5 (Society and ethics): Implement contextual knowledge and ethical principles to assess various societal issues related to common scientific and industrial practices. PO-6 (Environment and sustainability): Assess the impact of scientific approaches in environment with special emphasis on the need for sustainable development. PO-7 (Individual and teamwork): Function as an individual or as a member or leader in diverse teams, and in multidisciplinary settings. PO-8 (Communication): Communicate effectively, write reports and design documentation, make effective presentations, and give and receive clear instructions. PO-9 (Project management): Utilize knowledge and understanding of the chemical principles to manage projects of various magnitudes in multidisciplinary environments. PO-10 (Life-long learning): Identify the important aspects of Chemistry and other allied subjects for independent and life-long learning in the broader context of scientific and technological development.

Programme Specific Outcomes	PSO-1. To help students acquire advanced theoretical and practical knowledge in various fields of Chemical Sciences and allied subjects. PSO-2. To provide support to the students to become ethically and psychologically strong, socially conscious, expert professionals with independent thinking ability, leadership quality and excellent communication skills PSO-3. : To train the students to adopt into competitive work culture and flourish in industrial or academic environments.. PSO-4. To understand Analytical Chemistry and its applications through Various laboratory experiments. PSO-5. Use modern chemical tools, Models, Chem-draw, Charts and apparatus. PSO-6. Understand good laboratory practices and safety. PSO-7. Develop research oriented skills and thinking. PSO-8. Aware and good command on handling the sophisticated instruments/apparatus/equipments.

Course Outcomes M.Sc. Chemistry

Semester- I

Course	Outcomes
	After completion of these courses students should be able to:
PHYSICAL CHEMISTRY – I	CO-1. **Chemical Thermodynamics** CO-2. **Surface Chemistry** CO-3. **Chemical Kinetics** CO-4. **Electro Chemistry** CO-5. Macro Molecules
INORGANIC CHEMISTRY-I	CO-1. Reaction Mechanism of Transition Metal Complexes CO-2. Metal-Ligand Bonding CO-3. Electronic Spectra and Magnetic Properties of Transition Metal Complexes CO-4. Spectroscopic ground states, correlation, Orgel and Tanabe-Sugano diagrams for transition metalcomplexes

	CO-5. Metal π-Complexes
ORGANIC CHEMISTRY-I	CO-1. Types of mechanisms, types of reactions, thermodynamic and kinetic requirements, kinetic andthermodynamic control CO-2. Structure, stability and reactivity of carbocations, carbanions, free radicals, carbenes and nitrenes. CO-3. Aliphatic Nucleophilic Substitution CO-4. Aliphatic Electrophilic Substitution CO-5. Free Radical Reactions

SEMESTER - II	
ANALYTICAL CHEMISTRY	CO-1. Role of analytical chemistry. Classification of analytical methods-classical and instrumental. Types of instrumental analysis CO-2. Errors and Evaluation CO-3. Food Analysis CO-4. Analysis of Water Pollution CO-5. Analysis of Soil, Fuel, Body Fluids and Drugs
PHYSICAL CHEMISTRY-II	CO-1. Solid state chemistry CO-2. The Schrodinger equation and the postulates of quantum mechanics. Particle in three dimensional box CO-3. Linear Harminic oscillator, Harmonic Vibration Hermit differential equation and its solution through recursion relation CO-4. Variation method, Linear application to Harmonic oscillator CO-5. Huckle theory of conjugated systems
GROUP THEORY & SPECTROSCOPY	CO-1. **Symmetry and Group Theory in Chemistry** CO-2. Microwave Spectroscopy CO-3. Vibrational Spectroscopy CO-4. Nuclear Magnetic Resonance Spectroscopy CO-5. Electronic Spectroscopy
SEMESTER - III	
BIO-CHEMISTRY	CO-1.Understanding BIO-CHEMISTRY CO-2. Metal Ions in Biological Systems CO-3. Nitrogenase CO-4. Enzymes CO-5. Biotechnological Applications of Enzymes

ENVIRONMENTAL CHEMISTRY	CO-1. Understanding Environment CO-2. Hydrosphere CO-3. Soils CO-4. Analytical methods for measuring airpollutants. Continuous monitoring instruments CO-5. Chemical solutions to environmental problems, biodegradability, principles of decomposition
APPLICATIONS OF SPECTROSCOPY	CO-1. Understanding Electronic Spectroscopy CO-2. Hyperfine coupling, spin polarization for atoms and transition metal ions, spin-orbit coupling and significance of g-tensors CO-3. The contact and Pseudo contact shifts, factors affecting nuclear relaxation CO-4. Mössbauer Spectroscopy CO-5. Ultraviolet and Visible Spectroscopy

SEMESTER - IV	
INORGANIC CHEMISTRY SPECILISATION	
INORGANIC-II	CO-1. Alkyls and Aryls of Transition Metal CO-2. Compounds of Transition Metal-Carbon Multiple Bonds CO-3. Transition Metal π-Complexes CO-4. Homogeneous Catalysis CO-5. Fluxional Organometalilc Compounds
INORGANIC-III	CO-1. Metal Storage Transport and Biomineralization CO-2. Calcium in Biology CO-3. Metalloenzymes CO-4. Metals in Medicine CO-5. Supramolecular Chemistry
ORGANIC CHEMISTRY SPECILISATION	
ORGANIC-II	CO-1. Curve Crossing Model to Chemical Reactions CO-2. Principals of Reactivity CO-3. Kinetic Isotope Effect CO-4. Structural Effects on Reactivity CO-5. Supramolecular Chemistry
ORGANIC-III	CO-1. Pericyclic Reactions CO-2. Heterocycles CO-3. Synthesis and reactions of pyrylium salts and pyrones CO-4. Synthesis and reactions of diazines, triazines, tetrazines and thiazines CO-5. Vitamins
PHYSICAL CHEMISTRY SPECILISATION	
PHYSICAL-III	CO-1. Diffraction of X-rays by crystals CO-2. Metallic bonds CO-3. Electrically conducting polymers CO-4. Potential Energy Surfaces CO-5. Study of Fast Reactions

PHYSICAL-IV	CO-1. Super conductivity CO-2. Specific heat of solids CO-3. Surface chemistry surface films, BET isotherm for, multilayers & its derivation CO-4. Rate determining steps in diffusion controlled reactions and activation controlled reactions CO-5. Bronsted-Bjerrum equation

First Semester					
Paper Code	**Paper Name**	**Credit**	**Internal Marks**	**External Marks**	**Total Marks**
MSCCHE -101	INORGANIC CHEMISTRY-1	5	30	70	100
MSCCHE -102	ORGANIC CHEMISTRY -1	5	30	70	100
MSCCHE -103	PHYSICAL CHEMISTRY -1	5	30	70	100
MSCCHE -PR - 01	PRACTICAL-1	6		100	100
	TOTAL	**21**			**400**
Second Semester					
MSCCHE -201	ANALYTICAL CHEMISTRY	5	30	70	100
MSCCHE -202	GROUP THEORY & SPECTROSCOPY	5	30	70	100
MSCCHE-203	PHYSICAL CHEMISTRY -2	5	30	70	100
MSCCHE -PR - 02	PRACTICAL-2	6		100	100
	TOTAL	**21**			**400**
Third Semester					
MSCCHE -301	APPLICATIONS OF SPECTROSCOPY	5	30	70	100
MSCCHE -302	ENVIRONMENTAL CHEMISTRY	5	30	70	100
MSCCHE-303	BIO-CHEMISTRY	5	30	70	100
MSCCHE -PR - 03	PRACTICAL-3	6		100	100
	TOTAL	**21**			**400**
Fourth Semester (Specilization, choose any one group)					
Group A					
MSCCHE -401A	PHYSICAL CHEMISTRY-III	5	30	70	100
MSCCHE -402A	PHYSICAL CHEMISTRY-IV	5	30	70	100
MSCCHE-403A	PROJECT WORK	5			100
MSCCHE -PR-04A	PRACTICAL-4A	6			100
	TOTAL	**21**			**400**
Group B					
MSCCHE -401B	INORGANIC CHEMISTRY-II	5	30	70	100
MSCCHE -402B	INORGANIC CHEMISTRY-III	5	30	70	100
MSCCHE-403B	PROJECT WORK	5			100
MSCCHE -PR-04B	PRACTICAL-4B	6			100
	TOTAL	**21**			**400**
Group C					
MSCCHE -401C	ORGANIC CHEMISTRY-II	5	30	70	100
MSCCHE -402C	ORGANIC CHEMISTRY-III	5	30	70	100
MSCCHE-403C	PROJECT WORK	5			100
MSCCHE -PR-04C	PRACTICAL-4C	6			100
	TOTAL	**21**			**400**

SEMESTER I

PHYSICAL CHEMISTRY – I

Course Objectives:
To provide students with the knowledge of physical chemistry

CO-1. Chemical Thermodynamics

CO-2. Surface Chemistry
CO-3. Chemical Kinetics
CO-4. Electro Chemistry
CO-5. Macro Molecules

I. Chemical Thermodynamics (a) Partial molar properties in ideal gas mixture, Chemical Potential, its determination and variation with temperature and pressure, Gibb's Duhem equation. (b) Fugacity and activity its variation with 'T' and 'P', its determination. Fugacity of a gas mixture, Duhem, Margules equation and its application.

II. Statistical Thermodynamics Partition function and its significance, Relationship with thermodynamic functions, Translational, Rotational, Vibrational and Electronic partition function. Its application in the case of monoatomic and diatomic molecules.

III. Surface Chemistry Surface tension and Surface Free energy on liquids. Pressure difference across curved Surface (Laplace equation), Vapour pressure of droplets (Kelvin equation). Gibbs absorption isotherm, Estimation of surface area. (B.E.T equation), Unimolecular and bimolecular surface reations.

IV. Chemical Kinetics
Mechanism and Kinetics of consecutive and opposing reactions. Activated complex theory of Uni-molecular reaction. Mechanism and Kinetics of Photolysis of acetaldehyde and Photo dimerisation of Anthracene, Polymerization and Auto oxidation reaction. Homogeneous catalysis, Kinetic Enzyme catalysis, study of fast reactions by flow method and relaxation methods.

IV. Electro Chemistry
Electrode potential in terms of Chemical Potential and activity, Debye Huckle theory of conductance of electrolytic solution, its applications and limitations, Quantitative treatment of Debye Huckle Limiting law and its modification for finite size ions, effect of ion solvent interaction on activity coefficients, Butler-Volmer equation under equilibrium and non-equilibrium condition. Exchange current density Tafel Plot.

VI. Macro Molecules Types of Polymers, Kinetics and mechanism of Polymerization Molecular mass-number and mass average molecular mass, determinations of molecular mass by osmometry, viscosity and light scattering method.

Reference Books:

1. Physical Chemistry, P.W. Atkins, ELBS.
2. Quantum Chemistry, Ira N. Levine, Prentice Hall.
3. Chemical Kinetics, K. J. Laidler, Mcgraw-Hill.
4. Modern Electrochemistry Vol. I and Vol. II, J.O.M. Bockris and A.K.N. Reddy, Plenum.
5. Physcial chemistry by Puri, Sharma and Pathaniya

Course Outcomes

At the end of this course a candidate will be able to understand –

- Chemical Thermodynamics
- Surface Chemistry
- Chemical Kinetics
- Electro Chemistry
- Macro Molecules

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6	PO-7	PO-8	PO-9	PO-10
CO-1	3	3	2	1	1	1	1	3	3	3
CO-2	2	2	2	1	1	2	1	2	2	2
CO-3	2	2	3	2	1	2	1	2	2	2
CO-4	2	2	3	1	1	1	1	2	2	2
CO-5	3	3	2	2	1	1	1	3	3	3
CO-Average	2.40	2.40	2.40	1.40	1.00	1.40	1.00	2.40	2.40	2.40

3 is strongly mapped , 2 is moderately mapped, 1 is slightly mapped and 0 is non-mapped

INORGANIC CHEMISTRY-I

Course Objectives:

To provide students with the knowledge of In-organic chemistry

CO-1. Reaction Mechanism of Transition Metal Complexes

CO-2. Metal-Ligand Bonding

CO-3. Electronic Spectra and Magnetic Properties of Transition Metal Complexes

CO-4. Spectroscopic ground states, correlation, Orgel and Tanabe-Sugano diagrams for transition metal complexes

CO-5. Metal π-Complexes

I. Reaction Mechanism of Transition Metal Complexes

Energy profile of a reaction, reactivity of metal complexes, inert and labile complexes, kinetic application of valence bond and crystal field theories, kinetics of octahedral substitution, acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, direct and indirect evidences in favour of conjugate mechanism, anation reactions, reactions without metal ligand bond cleavage. Substitution reactions in square planar complexes, the trans effect, mechanism of the substitution reaction. Redox reactions, electron transfer reactions, mechanism of one electron transfer reactions, outer- sphere type reactions, cross reactions and Marcus-Hush theory, inner sphere type reactions

II. Metal-Ligand Bonding

Limitation of crystal field theory, molecular orbital theory, octahedral, tetrahedral and square planar complexes, p-bonding and molecular orbital theory.

III. Electronic Spectra and Magnetic Properties of Transition Metal Complexes

IV. Spectroscopic ground states, correlation, Orgel and Tanabe-Sugano diagrams for transition metal complexes (d^1-d^9 states), calculations of Dq, B and β parameters, charge transfer spectra, spectroscopicmethod of assignment of absolute configuration in optically active metal chelates andtheir stereochemical information, anomalous magnetic moments, magnetic exchange coupling and spincrossover.

V. Metal Clusters

Higher boranes, carboranes, metalloboranes and metallocarboranes. Metal carbonyl and halide clusters,compounds with metal-metal multiple bonds.

VI. Metal π-Complexes

Metal carbonyls, structure and bonding, vibrational spectra of metal carbonyls for bonding and structural elucidation, important reactions of metal carbonyls; preparation, bonding, structure and important reactions of transition metal nitrosyl, dinitrogen and dioxygen complexes: tertiary phosphine as ligand.

VII. Isopoly and Heteropoly Acids and Salts

- Spectroscopic ground states, correlation, Orgel and Tanabe-Sugano diagrams for transition metal complexes
- Metal π-Complexes

Reference Books:

1. Chemisiry of the Elements, N.N. Greenwood and A. Earnshow, Pergamon.
2. Advanced Inorganic Chemistry, F.A. Cotton and Wilkinson, John Wiley
3. Inorganic Chemistry, J.E. Huhey, Harpes & Row
4. Magnetochemistry, R.L. Cariin, Springer Vertag,
5. Comprehensive Coordination Chemistry eds., Q. Wilkinson, R.D. Gillars and J.A. Mc Cleverty, Pergamon.

Course Outcomes

At the end of this course a candidate will be able to understand –

- Reaction Mechanism of Transition Metal Complexes
- Metal-Ligand Bonding
- Electronic Spectra and Magnetic Properties of Transition Metal Complexes

INORGANIC CHEMISTRY-1

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6	PO-7	PO-8	PO-9	PO-10
CO-1	3	3	2	1	1	1	1	3	3	3
CO-2	2	2	2	1	1	2	1	2	2	2
CO-3	2	2	3	2	1	2	1	2	2	2
CO-4	2	2	3	1	1	1	1	2	2	2
CO-5	3	3	2	2	1	1	1	3	3	3
CO-Average	2.40	2.40	2.40	1.40	1.00	1.40	1.00	2.40	2.40	2.40

3 is strongly mapped , 2 is moderately mapped, 1 is slightly mapped and 0 is non-mapped

ORGANIC CHEMISTRY-I

Course Objectives:
To provide students with the knowledge of organic chemistry

CO-1. Types of mechanisms, types of reactions, thermodynamic and kinetic requirements, kinetic and thermodynamic control

CO-2. Structure, stability and reactivity of carbocations, carbanions, free radicals, carbenes and nitrenes.
CO-3. Aliphatic Nucleophilic Substitution
CO-4. Aliphatic Electrophilic Substitution
CO-5. Free Radical Reactions

I Reaction Mechanism: Structure and Reactivity

Types of mechanisms, types of reactions, thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond's postulate, 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.

Various type of steric strain and their influence on reactivity. Steric acceleration. Molecular measurements of steric effects upon rates, Steric LFER. Conformational barrier to bond rotation-spectroscopic detection of individual conformers. Acyclic and monocyclic systems. Rotation around partial double bonds. Winstein-Holness and Curtin-Hammett principle.

II Aliphatic Nucleophilic Substitution

The S_N2, S_N1, mixed S_N1 and S_N2 and SET mechanisms. Structural and electronic effects on S_N1 and S_N2 reactivity. Solvent effects. Kinetic isotope effects. Intramolecular assistance: Electrontransfer nature of S_N2 reaction.

The neighbouring group mechanism, neighbouring group participation by R and π-bonds, anchimeric assistance.

Classical and nonclassical carbocations, phenonium ions, norbornyl system, common carbocation rearrangements. Application of NMR spectroscopy in the detection ofcarbocations.
The S_Ni 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.

III Aliphatic Electrophilic Substitution

Elecrophilic reactivity, general mechanism. Bimolecular mechanisms- S_E2 and S_Ei. The S_E1 mechanism, electrophilic substitution accompanied by double bond shifts. Effect of substrates, leaving group and the solvent polarity on the reactivity.

Kinetic of SE2-Ar reaction. Structural effects on rates and selectivity.

IV Addition to Carbon-Carbon Multiple Bonds

Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, regio- and chemo-selectivity, orientation and reactivity. Addition to cyclopropane ring. Hydrogenation of double and triple bonds, hydrogenartion of aromatic rings. Hydroboration. Michael reaction. Sharpless asymmetric epoxidation.

V Addition to Carbon-Hetero Multiple Bonds

Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters and nitriles. Addition of Grignard reagents, Organozinc and Organolithium reagents to carbonyl and unsaturated carbonyl compounds. Mechanism of condensation reactions involving enolates- Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin and Stobbe reactions. Hydrolysis of esters and amides, ammonolysis of esters.

VI Aromatic Electrophilic Substitution

The arenium ion mechanism, orientation and reactivity, energy profile diagrams. The ortho/para ratio, ipso attack, orientation in other ring systems. Quantitative treatment of reactivity in substrates and electrophiles. Diazonium coupling, Vilsmeir reaction, Gattermann-Koch reaction.

VII Aromatic Nucleophilic Substitution

The S_NAr, S_N1, benzyne and $S_{RN}1$mechanisms. Reactivity - effect of substrate structure, leaving group and attacking nucleophile. The von Richter, Sommelet-Hauser, and Smiles rearrangements.

VIII Free Radical Reactions

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, auto-oxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts. Sandmeyer reaction. Free radical rearrangement. Hunsdiecker reaction.

Reference Books:

1. Advanced Organic Chemistry-Reactions, Mechanism and Structure, Jerry March, John Wi1ey.
2. Advanced Organic Chemistry, F. A. Carey and R. J. Sundberg, Plenum.
3. Organic Chemistry, R. T. Morrison and R. N. Boyd, Prentice-Hall.
4. Principles of Organic Synthesis, R. 0. C. Norman and J. M. Coxon, Blackle Academic & Professional.
5. Pericyclic Reactions, S. M. Mukherji, Macmillan, India.

6. Stereochemistry of Organic Compounds, D. Nasipuri, New Age international.

Course Outcomes

At the end of this course a candidate will be able to understand –

- Types of mechanisms, types of reactions, thermodynamic and kinetic requirements, kinetic and thermodynamic control
- Structure, stability and reactivity of carbocations, carbanions, free radicals, carbenes and nitrenes.
- Aliphatic Nucleophilic Substitution
- Aliphatic Electrophilic Substitution
- Free Radical Reactions

ORGANIC CHEMISTRY -1

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6	PO-7	PO-8	PO-9	PO-10
CO-1	2	3	2	1	1	1	1	3	3	2
CO-2	2	2	3	1	1	2	1	2	2	2
CO-3	2	2	3	2	1	2	1	3	2	2
CO-4	2	2	3	1	1	2	1	2	2	2
CO-5	3	3	2	2	1	1	2	3	3	2
CO-Average	2.20	2.40	2.60	1.40	1.00	1.60	1.20	2.60	2.40	2.00

3 is strongly mapped , 2 is moderately mapped, 1 is slightly mapped and 0 is non-mapped

PRACTICAL-I

INORGANIC CHEMISTRY

1. Cent per cent quantitative Analysis of Cement.
2. Estimation of the following:
(a) Magnesium by E.D.T.A. Methods (Volumetrically)
(b) Zinc by potassium ferrocyanide (Volumetrically)
(c) Nickel by Dimethylglyoxime (Gravimetrically)
(d) Managnese in steel by sodium bismuthate method.
3. A. Separation and determination of two metal ions Cu-Ni, Ni-Zn, Cu-Fe etc. involving volumetric and gravimetric methods.
B. Separation of cations and anions by a) Paper chromatography b) Column Chromatography.
4. Preparation of inorganic compounds:
(i) $[Cu(NH_3)_4]SO_4.H_2O$
(ii) $K_3[Fe(C_2O_4)_3]$
(iii) Prussian Blue, Turnbull's Blue
(iv) $[Ni(NH_3)_6]Cl_2$
(v) [Ni(dmg)2]

ORGANIC CHEMISTRY

5. Organic Qualitative
Identification of organic compounds containing one functional group using Chemical & Spectral Analysis
6 Separation, purification and identification of binary mixture (one liquid and one solid) involving TLC and Column Chronatography. Chemical tests and Functional group identification.
7 Preparation of organic compounds using methods not involving more than two steps.Some of the experiments listed below:
(i) Preparation of methyl Orange
(iv) Preparation of Martius yellow
(vi) Preparation of p-nitro aniline from acetanilide
(viii) Preparation of Cinnamic acid from Benzaldehyde

SEMESTER II

ANALYTICAL CHEMISTRY

Course Objectives:

To provide students with the knowledge of analytical chemistry

CO-1. Role of analytical chemistry. Classification of analytical methods-classical and instrumental. Types of instrumental analysis

CO-2. Errors and Evaluation

CO-3. Food Analysis

CO-4. Analysis of Water Pollution

CO-5. Analysis of Soil, Fuel, Body Fluids and Drugs

I Introduction

Role of analytical chemistry. Classification of analytical methods-classical and instrumental. Types of instrumental analysis. Selecting an analytical method. Neatness and cleanliness. Laboratory operations and practices. Analytical balance. Techniques of weighing, errors. Volumetric glassware-cleaning and calibration of glassware. Sample preparations - dissolution and decompositions. Gravimetric techniques. Selecting and handling of reagents. Laboratory notebooks. Safety in the analytical laboratory.

II Errors and Evaluation

Definition of terms in mean and median. Precision-standard deviation, relative standard deviation. Accuracy-absolute error, relative error. Types of error in experimental data-determinate (systematic), indeterminate (or random) and gross. Sources of errors and the effects upon the analytical results. Methods for reporting analytical data. Statistical evaluation of data-indeterminate errors. The uses of statistics.

III Food Analysis

Moisture, ash, crude protein, fat, crude fibre, carbohydrates, calcium, potassium, sodium and phosphate. Food adulteration-common adulterants in food, contamination of food stuffs. Microscopic examination of foods for adulterants. Pesticide analysis in food products. Extraction and purification of sample. HPLC. Gas chromatography for organophosphates. Thin-layer chromatography for identification of chlorinated pesticides in food products.

IV Analysis of Water Pollution

Origin of waste water, types, water pollutants and their effects. Sources of water pollution-domestic, industrial, agricultural soil and radioactive wastes as sources of pollution. Objectives *of* analysis-parameter for analysis-colour, turbidity, total solids, conductivity, acidity, alkalinity, hardness, chloride, sulphate, fluoride, silica, phosphates and different forms of nitrogen. Heavy metal pollution-public health significance of cadmium, chromium, copper, lead, zinc, manganese, mercury and arsenic. General survey of instrumental technique for the analysis of heavy metals in aqueous systems. Measurements of DO, BOD and COD. Pesticides as water pollutants and analysis. Water pollution laws and

standards.

V Analysis of Soil, Fuel, Body Fluids and Drugs

(a) Analysis of soil: moisture, pH, total nitrogen, phosphorus, silica, lime, magnesia, manganese, sulphur and alkali salts.

(b) Fuel analysis: solid, liquid and gas. Ultimate and proximate analysis-heating values grading of coal. Liquid fuels-flash point, aniline point, octane number and carbon residue. Gaseous fuels-producer gas and water gas-calorific value.

(c) Clinical chemistry: Composition of blood-collection and preservation of samples. Clinical analysis. Serum electrolytes, blood glucose, blood urea nitrogen, uric acid, albumin, globulins, barbiturates, acid and alkaline phosphatases. Immunoassay: principles of radio immunoassay (RIA) and applications. The blood gas analysis trace elements in the body.

(d) Drug analysis: Narcotics and dangerous drugs. Classification of drugs. Screening by gas and thin-layer chromatography and spectrophotometric measurements.

Reference Books:

1. Analytical Chemistry, G.D. Christian, J. Wiley.
2. Fundamentals of Analytical Chemistry, D.A. Skoog, D.M. West and F.J. Holler, W. B. Saunders.
3. Analytical Chemistry-Principles, J.H. Kennedy, W. B. Saunders.
4. Analytical Chemistry-Principles and Techniques, L.G. Hargis, Prentice Hall.
5. Principles of Instrumental Analysis, D.A. Skoog and J.L. Loary, W. B. Saunders.
6. Principles of Instrumental Analysis, D.A. Skoog, W. B. Saunders.
7. Quantitative Analysis, R.A. Day, Jr. and A.L. Underwood, Prentice Hall.
8. Environmental Solution Analysis, S.M. Khopkar, Wiley Eastern
9. Basic Concepts of Analytical Chemistry, S.M. Khopkar, Wiley Eastern
10. Handbook of Instrumental Techniques for Analytical Chemistry, F. Settle, Prentice Hall.
11. Analytical Chemistry, G.D. Christian, J. Wiley.

Course Outcomes

At the end of this course a candidate will be able to understand –

- Role of analytical chemistry. Classification of analytical methods-classical and instrumental. Types of instrumental analysis
- Errors and Evaluation
- Food Analysis
- Analysis of Water Pollution
- Analysis of Soil, Fuel, Body Fluids and Drugs

ANALYTICAL CHEMISTRY

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6	PO-7	PO-8	PO-9	PO-10
CO-1	3	3	2	2	2	3	3	3	1	2
CO-2	1	2	2	1	2	2	1	3	2	2
CO-3	3	2	2	2	2	3	1	2	1	1
CO-4	2	2	3	1	2	1	2	2	2	1
CO-5	3	3	2	2	1	3	1	3	1	3
CO-Average	2.40	2.40	2.20	1.60	1.80	2.40	1.60	2.60	1.40	1.80

PHYSICAL CHEMISTRY-II

Course Objectives:

To provide students with the knowledge of physical chemistry

CO-1. Solid state chemistry

CO-2. The Schrodinger equation and the postulates of quantum mechanics. Particle in three dimensional box

CO-3. Linear Harminic oscillator, Harmonic Vibration Hermit differential equation and its solution through recursion relation

CO-4. Variation method, Linear application to Harmonic oscillator

CO-5. Huckle theory of conjugated systems

I Solid state chemistry

Perfect and imperfect crystals, intrinsic and extrinsic defects, line defects, plane defects, Vaccancies-schottky and Frenkel defect. Non-stochiometric defects.

II Introduction of Quantum mechanics

The Schrodinger equation and the postulates of quantum mechanics. Particle in three dimensional box, Hermitian operators, properties of operators, Angular momentum operator, their Eigen function and Eigen values, Theorem of operators.

III Exactly Soluble System

Linear Harminic oscillator, Harmonic Vibration Hermit differential equation and its solution through recursion relation, Hermit polynomial. H-like atoms, separation of r, θ, ϖ equation. Laguerre and associated Laguerre polynomial. Legendre polynomial equation and their solution. the rigid rotor.

IV Approximate Method

Variation method, Linear application to Harmonic oscillator, perturbation method, first order perturbation, Application to He-atom.

Huckle theory of conjugated systems, bond order and charge density-its calculation. Application to ethylene and butadiene.

Reference Books:

1. Physical Chemistry, P.W. Atkins, ELBS.
2. Quantum Chemistry, Ira N. Levine, Prentice Hall.
3. Chemical Kinetics, K. J. Laidler, Mcgraw-Hill.
4. Modern Electrochemistry Vol. I and Vol. II, J.O.M. Bockris and A.K.N. Reddy, Plenum.
5. Physcial chemistry by Puri, Sharma and Pathaniya

Course Outcomes

At the end of this course a candidate will be able to understand –

- Solid state chemistry
- The Schrodinger equation and the postulates of quantum mechanics. Particle in three dimensional box
- Linear Harminic oscillator, Harmonic Vibration Hermit differential equation and its solution through recursion relation
- Variation method, Linear application to Harmonic oscillator
- Huckle theory of conjugated systems

PHYSICAL CHEMISTRY -2

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6	PO-7	PO-8	PO-9	PO-10
CO-1	3	3	2	2	3	3	2	3	3	3
CO-2	2	3	2	2	3	2	1	2	1	2
CO-3	2	3	3	2	3	2	2	2	1	2
CO-4	2	2	3	1	1	1	1	1	1	2
CO-5	3	3	2	2	1	3	1	3	3	3
CO-Average	2.40	2.80	2.40	1.80	2.20	2.20	1.40	2.20	1.80	2.40

3 is strongly mapped , 2 is moderately mapped, 1 is slightly mapped and 0 is non-mapped

GROUP THEORY & SPECTROSCOPY

Course Objectives:

To provide students with the knowledge of group theory & spectroscopy

CO-1. **Symmetry and Group Theory in Chemistry**

CO-2. Microwave Spectroscopy

CO-3. Vibrational Spectroscopy

CO-4. Nuclear Magnetic Resonance Spectroscopy

CO-5. Electronic Spectroscopy

I Symmetry and Group Theory in Chemistry

Symmetry elements and symmetry operation, definitions of group, subgroup, relation between orders of a finite group and its subgroup. Conjugacy relation and classes. Point symmetry group. Schonflies symbols, representations of groups by matrices (representation for the Cn, Cnv, Cnh. Dnh etc. groups to be worked out explicitly). Character of a representation. The great orthogonality theorem (without proof) and its importance. Character tables and their use; spectroscopy.

II Microwave Spectroscopy

Classification of molecules, rigid rotor model, effect of isotopic substitution on the transition frequencies, intensities, non-rigid rotor. Stark effect, nuclear and electron spin interaction and effect of external field. Applications.

III Vibrational Spectroscopy

A. Infrared Spectroscopy

Review of linear harmonic oscillator, vibrational energies of diatomic molecules, zero point energy, force constant and bond strengths; anharmonicity, Morse potential energy diagram, vibration-rotation spectroscopy, P,Q,R branches. Breakdown of Oppenheimer approximation; vibrations of polyatomic molecules. Selection rules, normal modes of vibration, group frequencies, overtones, hot bands, factors affecting the band positions and intensities, far IR region, metal-ligand vibrations, normal co-ordinate analysis,

B. Raman Spectroscopy

Classical and quantum theories of Raman effect. Pure rotational, vibrational and vibrational-rotational Raman spectra, selection rules, mutual exclusion principle. Resonance Raman spectroscopy, coherent anti Stokes Raman spectroscopy (CARS).

IV Magnetic Resonance Spectroscopy

A. Nuclear Magnetic Resonance Spectroscopy

Nuclear spin, nuclear resonance, saturation, shielding of magnetic nuclei, chemical shift, deshielding, spin-spin interactions, factors influencing coupling constant "j" Classification (AXB, AMX, ABC, A_2B_2 etc.), spin decoupling; basic ideas about instrument, NMR studiesof nuclei other than proton-^{13}C, ^{19}F and ^{31}P. FT NMR, advantages of FT NMR.

B. Nuclear Quadrupole Resonance Spectroscopy

Quadrupole nuclei, quadrupole moments, electric field gradient, coupling constant, splitting. Applications.

C. Electron Spin Resonance Spectroscopy

Basic principles, zero field splitting and Kramer's degeneracy, factors affecting the 'g' value. Isotropic and anisotropic hyperfine coupling constants, spin Hamiltonian, spin densities and Mc Connell relationship, measurement techniques, applications.

V Electronic Spectroscopy

A. Atomic Spectroscopy

Energies of atomic orbitals, vector representation of momenta and vector coupling, spectra of hydrogen atom and alkali metal atoms.

B. Molecular Spectroscopy

Energy levels, molecular orbitals, vibronic transitions, vibrational progressions and geometry of the excited states, Franck-Condon principle, electronic spectra of polyatomic molecules. Emission spectra; radiative and non-radiative decay, internal conversion, spectra of transition metal complexes, charge-transfer spectra.

VI X-ray Diffraction

Bragg condition, -Miller indices, Laue method, Bragg method, Debye-Scherrer method of X-ray structural analysis of crystals, index reflections, identification of unit cells from systematic absences in diffraction pattern. Structure of simple lattices and X-ray intensities, structure factor and its relation to intensity and electron density, phase problem. Description of the procedure for an X-ray structure analysis, absolute configuration of molecules, Ramchandran diagram.

Reference Books:

1 Applied Electron Spectroscopy lor Chemical Analysis Ed. H. Windawi and F.L. Ho. Wiley Interscience.
2 NMR, NOR, EPR and Massbauer Spectroscopy in Inorganic Chemistry, R.V. Parish, Ellis Harwood.
3 PhysicaI' Methods in Chemistry, R.S. Drago, Saunders College.
4 Chemical Applications of Group Theory, F. A. Cotton.
5 Introduction to Molecular Spectroseopy, Q.M. Barrow, McCraw Hill.
6 Basic Principles of Spectroscopy. R. Chang, McOraw Hill.
7 Theory and Applications of UV Spectroscopy, H.H. Jatie and M. Orehin, IBH-Oxford.
8 Introduction to Photoelectron Spectroscopy, P. K. Ghosh, John Wiley.
9 Introduction to Magnetic Resonance, A. Carrington and A.D. Maclachalan, Harper & Row.
10 Modern Speciroscopy, J.M. Hollas, John Wiley.

Course Outcomes

At the end of this course a candidate will be able to understand –

- Symmetry and Group Theory in Chemistry
- Microwave Spectroscopy
- Vibrational Spectroscopy
- Nuclear Magnetic Resonance Spectroscopy

Electronic Spectroscopy

GROUP THEORY & SPECTROSCOPY										
	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6	PO-7	PO-8	PO-9	PO-10
CO-1	3	3	2	2	1	3	1	3	3	3
CO-2	3	2	2	1	1	2	1	3	2	3
CO-3	2	1	3	2	2	2	2	2	2	1
CO-4	3	2	3	1	1	1	1	1	2	2
CO-5	3	1	2	2	1	3	1	3	1	3
CO-Average	2.80	1.80	2.40	1.60	1.20	2.20	1.20	2.40	2.00	2.40

3 is strongly mapped , 2 is moderately mapped, 1 is slightly mapped and 0 is non-mapped

PRACTICAL-II

1. **Measurement of density of gases and vapours**
   (a) Victor Meyer's Method Determination of Molecular weight of Acetone, Chloroform, Benzene, (Mixture).
   (b) Duma's Method Determination of molecular weight of acetone, Carbon-Tetrachloride.
2. **Determination of Molecular weight of substances**
   (a) Beckmann's freezing point Method
   (b) Beckmann's Boiling point method.
3. **Viscosity of liquids and solution by ostwald tube**
   Determination of percentage composition of a mixture of two liquids.
4. **Surface Tension of liquids and solutions**
   (a) Study of the effect of conc. on surface tension of acetic acid and Sodium chloride solutions.
   (b) Determination of Parachor.
5. **Thermochemistry**
   (a) Determination of water equivalent of a calorimeter
   (b) Determination of the Heat of Neutralization of :
      (i) Strong acid and strong base (HCl and NaOH)
      (ii) Weak acid and strong base (NaOH and CH_3COOH).
   (c) Determination of Heat of solution of Potassium Nitrate
   (d) Determination of basicity of succinic Acid by Thermochemical Method.
6. **Order of Reaction**
   (a) Determination of the rate constant of hydrolysis of an ester with an acid (Methyl acetate and HCl).
   (b) Determination of the rate constant of saponification of ethyl acetate by NaOH.
7. **Partition Co-efficient**
   (a) Determination of partition coefficient of:
      (i) Benzoic acid between water and Benzene
      (ii) Iodine between water and carbon tetrachloride
9. **Conductivity**
   (a) Determination of cell constant
   (b) Determination of equivalent conductivity of weak acid (acetic and succinic acid) at several concentrations and calculation of the dissociation constant of the acid
   (c) Determination of the basicity of an acid (citric acid and oxalic acid)
   (d) Titration of:
      (i) strong acid and strong base (HCl and NaOH)
      (ii) weak acid and strong base (CH_3COOH and NaOH)

SEMESTER III

BIO-CHEMISTRY

Course Objectives:

To provide students with the knowledge of Bio-chemistry

CO-1.Understanding BIO-CHEMISTRY

CO-2. Metal Ions in Biological Systems

CO-3. Nitrogenase

CO-4. Enzymes

CO-5. Biotechnological Applications of Enzymes

GROUP-A (Bioinorganic Chemistry)

I Metal Ions in Biological Systems

Essential and trace metals. Na^+/K^+ Pump

Role of metals ions in biological processes,

II Bioenergetics and ATP Cycle

DNA polymerisation, glucose storage, metal complexes in transmission of energy; chlorophylls, photosystem I and photosystem II in cleavage of water. Model systems.

III Transport and Storage of Dioxygen

Heme proteins and oxygen uptake, structure and function of hemoglobin, myoglobin, hemocyanins and hemerythrin, model synthetic complexes of iron, cobalt and copper.

IV Electron Transfer in Biology

Structure and function of metalloproteins in electron transport processes - cytochromes and ion-sulphur proteins, synthetic models

V Nitrogenase

Biological nitrogen fixation, molybdenum nitrogenase, spectroscopic and other evidence, other nitrogenases model systems.

GROUP-B (Bioorganic Chemistry)

I Enzymes and Mechanism of Enzyme Action

Basic considerations. Proximity effects and molecular adaptation.

Enzymes

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 Koshtand's induced fit hypothesis, concept and identification of active site by the use of inhibitors, affinity labeling and enzyme modification by site-directed mutagenesis. Enzyme kinetics, Michaelis-Menten and Lineweaver-Burk plots, reversible and irreversible Inhibition.

Mechanism of Enzyme Action

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

II Kinds of Reactions Catalysed by Enzymes

Nucleophilic displacement on a phosphorus atom, multiple displacement reactions and the coupling of ATP cleavage to endergonic processes. Addition and elimination reactions, enolic intermediates in isomerization reactions, p-cleavage and condensation, some isomerization and rearrangement reactions. Enzyme catalyzed carboxylation and decarboxylation.

III Co-Enzyme Chemistry

Enzyme Models. Cofactors as derived from vitamins, coenzymes, prosthetic groups, apoenzymes. Structure and biological functions of coenzyme A, thiamine pyrophosphate, pyridoxal phosphate, NAD^+, $NADP^+$ FMN, FAD, lipolc acid, vitamin B_{12}. Mechanisms of reactions catalyzed by the above cofactors.

IV Biotechnological Applications of Enzymes

Large-scale production and purification of enzymes, techniques and methods of immobilization of enzymes, effect of immobilization on enzyme activity, application of immobilized enzymes, use of enzymes in food and drink industry-brewing and cheese- making, syrups from corn starch, enzymes as targets for drug design. Clinical uses of enzymes, enzyme therapy, enzymes and recombinant DNA technology.

Reference Books:

1.Principles of Bioinorganic Chemistry, S.J. Lippard and J.M. Berg, University Science Books.
2.Bioinorganic Chemistry, I. Bertini, H.B. Gray, S.J. Lippard and J.S. Valentine, University Science Books.
3. Inorganic Biochemistry vols I and II. ed. G.L. Eichhorn, Elsevier.
4. Progress in Inorganic Chemistry, Vols 18 and 3S ed. J.J. Lippard, Wiley.
5. Bioorganic Chemistry: A Chemical Approach to Enzyme Action, Hermann Dugas and C. Penny, Springer-Verlag.
6. Understanding Enzymes, Trevor Palmer, Prentice Hall.
7. Enzyme Chemistry: Impact and Applications, Ed. Collin J Suckling, Chapman and Hail.
8. Enzyme Mechanisms Ed, M. 1. Page and A. Williams, Royal Society of Chemistry.
9.Fundamentals of Enzymology, N.C. Price and L. Slovens, Oxford University Press.
10. Immobilized Enzymes: An Introduction and Applications In Biotechnology, Michael 0. Trevan, John Wiley.
11. Enzymatic Reaction Mechanisms, C. Walsh, W. H. Freeman.
12. Enzyme Structure and Mechanism, A Fersht, W.H. Freeman.
13. Biochemistry: The Chemical Reactions of Living Cells, D. E. MeUler, Academic Press.

Course Outcomes

At the end of this course a candidate will be able to understand –

- Understanding BIO-CHEMISTRY
- Metal Ions in Biological Systems
- Nitrogenase
- Enzymes
- Biotechnological Applications of Enzymes

BIO-CHEMISTRY

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6	PO-7	PO-8	PO-9	PO-10
CO-1	3	3	2	2	1	3	1	3	3	3
CO-2	3	2	1	1	1	3	3	2	2	3
CO-3	3	2	1	2	2	2	3	3	2	2
CO-4	2	1	1	1	2	1	1	1	3	2
CO-5	3	1	2	2	1	3	1	3	3	3
CO-Average	2.80	1.80	1.40	1.60	1.40	2.40	1.80	2.40	2.60	2.60

ENVIRONMENTAL CHEMISTRY

Course Objectives:

To provide students with the knowledge of environmental chemistry

CO-1. Understanding Environment

CO-2. Hydrosphere

CO-3. Soils

CO-4. Analytical methods for measuring airpollutants. Continuous monitoring instruments

CO-5. Chemical solutions to environmental problems, biodegradability, principles of decomposition

I Environment

Introduction. Composition of atmosphere, vertical temperature, heat budget of the earth atmospheric system, vertical stability atmosphere. Biogeochemical cycles of C, N, P, S and 0. Biodistribution of elements.

II Hydrosphere

Chemical composition of water bodies-lakes, streams, rivers and wet lands etc. Hydrological cycle. Aquatic pollution - inorganic, organic, pesticide, agricultural, industrial and sewage, detergents, oil spills and oil pollutants. Water quality parameters - dissolved oxygen, biochemical oxygen demand, solids, metals, content of chloride, sulphate, phosphate, nitrate and micro-organisms. Water quality standards. Analytical methods for measuring BOD, DO, COD, F, Oils, metals (As, Cd, Cr, Hg, Pb, Se etc.), residual chloride and chlorine demand. Purification and treatment of water.

III Soils

Composition, micro and macro nutrients, Pollution'- fertilizers, pesticides, plastics and metals. Waste treatment.

IV Atmosphere

Chemical composition of atmosphere - particles, ions and radicals and their formation. Chemical and photochemical reactions in atmosphere, smog formation, oxides of N, C, S, 0 and their effect, pollution by chemicals, petroleum, minerals, chlorofluorohydrocarbons. Green-house effect, acid rain, air pollution controls and their chemistry. Analytical methods for measuring air pollutants. Continuous monitoring instruments.

V Industrial Pollution

Cement, sugar, distillery, drug, paper and pulp, thermal power plants, nuclear power plants, metallurgy. Polymers, drugs etc. Radionuclide analysis. Disposal of wastes and their management.

VI Environmental Toxicology

Chemical solutions to environmental problems, biodegradability, principles of decomposition, better industrial processes. Bhopal gas tragedy, Chernobyl, Three mile island, Sewozo and Minamata disasters.

Reference Books:

1. Environmental Chemistry, S. E. Manahan, Lewis Publishers.
2. Environmental Chemistry, Sharma & Kaur, Krishna Pubilshers.
3. Environmenlal Chemistly, A. K. De, Wiley Easlem.
4. Environmental Pollution Analysis, S.M. Khopkar, Wiley Eastern
5. Standard Method of Chemical Analysis, FJ. Weleher Vol. III. Van Nostrand Reinhold Co.
6. Environmental Toxicology, Ed. J. Rose, Gordon and Breach Science Publication.

Course Outcomes

At the end of this course a candidate will be able to understand –

- Understanding Environment
- Hydrosphere
- Soils
- Analytical methods for measuring airpollutants. Continuous monitoring instruments
- Chemical solutions to environmental problems, biodegradability, principles of decomposition

ENVIRONMENTAL CHEMISTRY

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6	PO-7	PO-8	PO-9	PO-10
CO-1	3	3	2	2	1	3	1	3	2	1
CO-2	1	2	2	1	2	3	3	2	2	2
CO-3	2	1	1	2	1	2	2	2	2	2
CO-4	2	2	3	1	1	1	1	2	2	1
CO-5	2	1	2	1	3	2	1	3	2	3
CO-Average	2.00	1.80	2.00	1.40	1.60	2.20	1.60	2.40	2.00	1.80

3 is strongly mapped , 2 is moderately mapped, 1 is slightly mapped and 0 is non-mapped

APPLICATIONS OF SPECTROSCOPY

Course Objectives:

To provide students with the knowledge of applications of spectroscopy

CO-1. Understanding Electronic Spectroscopy

CO-2. Hyperfine coupling, spin polarization for atoms and transition metal ions, spin-orbit coupling and significance of g-tensors

CO-3. The contact and Pseudo contact shifts, factors affecting nuclear relaxation

CO-4. Mössbauer Spectroscopy

CO-5. Ultraviolet and Visible Spectroscopy

Inorganic Chemistry

I Electronic Spectroscopy

Electronic Spectral Studies for d^1- d^9 systems in octahedral, tetrahedral and square planer complexes,

II Vibrational Spectroscopy

Symmetry and shapes of AB_2, AB_3, AB_4, AB_5 and AB_6, mode of bonding of ambidentate ligands, nitrosyl, ethylenediamine and diketonato complexes, application of resonance. Raman spectroscopy and its applications.

III Electron Spin Resonance Spectroscopy

Hyperfine coupling, spin polarization for atoms and transition metal ions, spin-orbit coupling and significance of g-tensors, application to transition metal complexes (having one unpaired electron) including biological systems and to inorganic free radicals such as PH_4, $F_2^-$and $[BH_3]^-$.

IV Nuclear Magnetic Resonance of Paramagnetic Substances in Solution

The contact and Pseudo contact shifts, factors affecting nuclear relaxation, some applications including biochemical systems, an overview of NMR of metal nuclide with emphasis on ^{195}Pt and ^{119}Sn NMR.

V Mössbauer Spectroscopy

Basic principles, spectral parameters and spectrum display. Application of the technique to the studies of (1) bonding and structures of Fe^{+2} and Fe^{+3} compounds including those of intermediatespin, (2) Sn^{+2} and Sn^{+4} compounds - nature of M-L bond, coordination number, structure and (3) detection of oxidation state and inequivalent MB atoms.

Organic Chemistry

I Ultraviolet and Visible Spectroscopy

Various electronic transitions (185-800 nm), Beer—Lambert law, effect of solvent on electronic transitions, ultraviolet bands for carbonyl compounds, unsaturated carbonyl compounds, dienes,

conjugated polyenes. Fieser-Woodward rules for conjugated dienes and carbonyl compounds, ultraviolet spectra of aromatic and heterocyclic compounds.

II Infrared Spectroscopy

Instrumentation and sample handling. Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols and amines. Detailed study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides, acids, anhydrides, lactones, lactams and conjugated carbonyl compounds).Effect of hydrogen bonding

and solvent effect on vibrations frequencies, overtones, combination bands and Fermi resonance. FT IR. IR of gaseous, solids and polymeric materials.

III Nuclear Magnetic Resonance Spectroscopy

PMR Spectroscopy

General introduction and definition, chemical shift, spin-spin interaction, shielding mechanism, chemical shift values and correlation for protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic) and other nuclei (alcohols, phenols, enols, carboxylic acids, amines, amides & mercapto), chemical exchange, effect of deuteration, solvent effects. Fourier transform technique.

Carbon-13 NMR Spectroscopy

General considerations, chemical shift (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbon), coupling constants. Two dimension NMR spectroscopy - COSY, NOESY, DEPT, INEPT, APT and INADEQUATE techniques.

IV Mass Spectrometry

Introduction, ion production - El, Cl, FD and FAB, factors affecting fragmentation, ion analysis, ion abundance. Mass spectral fragmentation of organic compounds, common functional groups, molecular ion peak, metastable peak, McLafferty rearrangement. Nitrogen rule. High resolution mass spectrometery. Examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

Reference Books:

1. Physical Methods lor Chemistry, R.S. Drago, Saunders Company.
2. Structural Melhods in Inorganic Chemistry, E.A.V. Ebsworth, D.W.H. Rankin and S. Cradock, ELBS.
3. Infrared and Raman Spectra: Inorganic and Coordination Compounds, K. Nakamoto, Wiley.
4. Progress in Inorganic Chemistry vol., 8, ed., F.A. Cotton, vol., 15, ed. S.J. Lippard, Wiley.
5. Transition Metal Chemistry eA R.L. Carlin voi. S, Dekker
6. Inorganic Elecironie Speciroscopy,. A.P.B. Lever, Elsevier.
7. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R.V. Parish, Ellis Horwood.
8. Practical NMR Spoctroacopy, M.L Martin, J.J. Delpeuch and Q.J. fArtin, Heyden.
9. Spedrometric identitication of Organic Compounds, R. M. Silverstein, Q. C. gassier and T. C. Morrill, John Wiley
10. lnirodlJCtion lo NMR Spectroscopy. R. J. Abraham, J. Fisher and P. Loftus, Wiley.
11. Application of Spectroscopy of Oiganic Compounds, J. R. Dyer, Prentice Hail.
12. Spectroscopic Methods in Organic Chemistry, D. H. Williams, 1. Fleming, Tala McGraw-Hill.

Course Outcomes

At the end of this course a candidate will be able to understand –

- Understanding Electronic Spectroscopy
- Hyperfine coupling, spin polarization for atoms and transition metal ions, spin-orbit coupling and significance of g-tensors
- The contact and Pseudo contact shifts, factors affecting nuclear relaxation
- Mössbauer Spectroscopy
- Ultraviolet and Visible Spectroscop**PPLICATIONS OF SPECTROSCOPY**

APPLICATIONS OF SPECTROSCOPY

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6	PO-7	PO-8	PO-9	PO-10
CO-1	2	3	2	2	3	3	1	3	3	3
CO-2	2	2	3	1	3	2	2	2	2	2
CO-3	2	2	3	2	3	2	1	2	2	2
CO-4	2	2	3	1	1	1	3	1	2	2
CO-5	3	3	2	2	1	3	1	3	3	1
CO-Average	2.20	2.40	2.60	1.60	2.20	2.20	1.60	2.20	2.40	2.00

3 is strongly mapped , 2 is moderately mapped, 1 is slightly mapped and 0 is non-mapped

PRACTICAL-III

1. Experiments-I (Lab-work)

Group-A: Estimation of following in water

(a) Ca (b) Fe (c) Mg
(d) Chemical oxygen demand (COD)
(e) Biochemical oxygen demand (BOD) &
(f) Dissolved oxygen (DO)

Group-B: Analysis of soil for the followings

(a) Ca (b) Mg (c) Total nitrogen
(d) Carbonate (e) Organic matter (f) Ammonia & (g) Nitrate nitrogen

2. Experiments-II (Field-work)

Group-C: Field work consist of

1. Visit to some nearby areas (river, villages, industrial area) for collection of water & soil samples
2. Analysis of sample with reference to pollution and
3. Submission of report of field work

3. Note book and attendance

4. viva-voce

SEMESTER IV

GENERIC/ DISCIPLINE CENTRIC ELECTIVE

PHYSICAL CHEMISTRY -III

Course Objectives:

To provide students with the knowledge of physical chemistry

CO-1. Diffraction of X-rays by crystals

CO-2. Metallic bonds

CO-3. Electrically conducting polymers

CO-4. Potential Energy Surfaces

CO-5. Study of Fast Reactions

I Diffraction of X-rays by crystals

Debye Scherrer mechod, indexing powder pattern for cubic and tetragonal crystals, rotating crystal method, Fourier transform and reciprocal lattices, Bragg equation in reciprocal lattice, neutron diffraction.

II Metallic bonds

Free electron theory, band theory, Fermi level, Brillouin zone, wave function for electrons in solids, metallic conductors, insulator, semiconductors (intrinsic & extrinsic), properties of junctions.

III Polymer

Polymer solution, thermodynamics of polymer solutions, molar mass and molar mass distribution, methods of measuring molar masses, micelle formation and hydrophobic interaction.

IV Electrically conducting polymers

Electrically conducting polymers electrochemical polymerization, band structure of polymers, mechanism of conduction in polymers, doping of polymers, application of conduction polymers.

V Potential Energy Surfaces

Mechanism of activation, potential energy surface for three atom reaction, Potential energy curve for successive reactions, Properties of potential energy surfaces, Inter conversion of translational and vibrational energies, Combination of atoms, Orthopara conversion, Activated state of three atom and four atom reactions, Potential energy profile, reaction co-ordinate, Transmission co-efficient, non-adiabatic reaction.

VI Study of Fast Reactions

Photo physical Chemistry-Flash Photolysis, Relaxation technique, Nuclear Magnetic Resonance Method, Molecular Beam and Shock-tube Kinetics, Flow method. Reactions of Protons, Electrons metal ions.

Course Outcomes

At the end of this course a candidate will be able to understand –

- Diffraction of X-rays by crystals
- Metallic bonds
- Electrically conducting polymers
- Potential Energy Surfaces
- Study of Fast Reactions

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6	PO-7	PO-8	PO-9	PO-10
CO-1	2	3	3	2	1	3	1	3	3	3
CO-2	2	3	3	3	3	2	1	2	2	2
CO-3	2	3	3	2	1	3	3	2	3	3
CO-4	2	2	3	1	3	3	1	3	3	2
CO-5	3	3	3	2	1	3	3	3	3	3
CO-Average	2.20	2.80	3.00	2.00	1.80	2.80	1.80	2.60	2.80	2.60

3 is strongly mapped , 2 is moderately mapped, 1 is slightly mapped and 0 is non-mapped

GENERIC/ DISCIPLINE CENTRIC ELECTIVE

PHYSICAL CHEMISTRY -IV

Course Objectives:

To provide students with the knowledge of physical chemistry

CO-1. Super conductivity

CO-2. Specific heat of solids

CO-3. Surface chemistry surface films, BET isotherm for, multilayers & its derivation

CO-4. Rate determining steps in diffusion controlled reactions and activation controlled reactions

CO-5. Bronsted-Bjerrum equation

I **Super conductivity**

Super conductivity meissner effect, microscopic theory of superconductivity, conventional organic and high temp, superconductors, fullerenes, applications of superconductors.

Transformation in crystals - thermodynamics of transformation, order-disorder transitions, martensitic transition, polymorphic transformation

II **Specific heat of solids**

Specific heat of solids classical theory, quantum theory of specific heats-Einstein and Debye theories, characteristic temp and its calculation, T-law. Solid state reactions, laws governing nucleation, homogeneous and heterogenous nucleation, thermodynamic barrier.

III **Polymer liquid crystal**

Polymer liquid crystal nematic, cholesteric and smectic phases, liquid crystalline order of the main chain and of the side groups in polymers, synthesis and properties of polymer liquid crystals, liquid crystalline order in biological materials.

IV **Surface chemistry**

Surface chemistry surface films, BET isotherm for, multilayers & its derivation, kinetics of surface processes, unimolecular and bimolecular surface reactions, electrocapillarity, electrokinetic effects, statistical mechanics of adsorption, Colloids.

V **Kinetics of Condensed Phase Reactions**

Rate determining steps in diffusion controlled reactions and activation controlled reactions, Stokes-Einstein equation and dependence of rate constant on co-efficient of viscosity of medium, Kinetics of ionic reactions in solution-electrostatic contribution to free energy in single and double spherical models of activated complex, entropy of activation for ion-ion reactions; Kinetics of dipole-dipole reaction, ion-dipole reaction, dependence of rate constant on ionic strength and dielectric constant of medium, Bronsted-Bjerrum equation.

Reference Books:

1. Crystallography - Philips
2. Solid State chernistry-Garner (Butterworth; London)
3. Solid State Chemistry -D.K.Chakraborty (New Age int Publication)
4. Solid State Chemistry- N. BHannay (Prentice Hall, New Jersay)
5. Physical Chemistry- Waller J. Moore
6. Principles of polymer chemistry Cornell , P. J. Flory (Univ. Press)
7. Handbook of Conducting Polymers Vol I & II" T A. Skolhia

Course Outcomes

At the end of this course a candidate will be able to understand –

- Super conductivity
- Specific heat of solids
- Surface chemistry surface films, BET isotherm for, multilayers & its derivation
- Rate determining steps in diffusion controlled reactions and activation controlled reactions
- Bronsted-Bjerrum equation

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6	PO-7	PO-8	PO-9	PO-10
CO-1	3	3	2	2	1	3	1	3	3	3
CO-2	3	2	3	1	3	2	1	3	2	2
CO-3	3	2	3	2	1	2	1	2	2	3
CO-4	3	2	3	1	3	3	3	3	3	2
CO-5	3	3	2	2	1	3	1	3	3	1
CO-Average	3.00	2.40	2.60	1.60	1.80	2.60	1.40	2.80	2.60	2.20

3 is strongly mapped , 2 is moderately mapped, 1 is slightly mapped and 0 is non-mapped

GE/DC PRACTICAL:

PRACTICAL–IV A
PHYSICAL CHEMISTRY PRACTICAL

1. **Conductometry**
   a. To determine the solubility and solubility product of a sparingly soluble salt
   b. To verify Onsager equation for a uni-univalent electrolyte in aqueous solution
   c. To titrate a mixture of HCl, CH_3COOH and $CuSO_4$ with NaOH
   d. To determine the rate constant of saponification of an ester by NaOH.

2. **Determination of Equivalence conductance of following strong electrolyte:**
   a. KCl
   b. NaCl
   c. AgNO3
   d. HCl
   e. KNO3

3. **Potentiometry**
   a. To determine the solubility and solubility product of AgCl in water
   b. To determine the E^0 of Zn/Zn^{++}, Cu/Cu^{++} electrodes.
   c. To determine the basicity of a polybasic acid and its dissociation constant.
   d. To investigate the complex formed between $CuSO_4$ and NH_3.

4. **Polarography**
   a. Estimation of Pb^{2+} and Cd^{2+}/ Zn^{2+} and Ni^{2+} metal ions in a mixture of Pb^{2+} and Cd^{2+}/ Zn^{2+} and Ni^{2+} by polarography.
   b. Determination of dissolved oxygen in aqueous solution of organic solvents.

5. **Chemical Kinetics**
   a. Determination of relative strengths of HCl and H_2SO_4 (k_1 / k_2) for the hydrolysis of methylacetate.
   b. Determination of relative strengths of HNO_3 and H_2SO_4 (k_1 / k_2) for the hydrolysis ofmethyl acetate.

c. To study the kinetics of alkaline hydrolysis of an ester in aquo-organic solvent system with respect to effect of solvent composition and dielectric constant on rate constant.
d. To determine the rate constant of the reaction between $K_2S_2O_8$ and KI at two differenttemp. and hence to determine the energy of activation of the reaction.

6. Thermochemistry

a. Determination of basicity of a polybasic acid.
b. Determination of heat of displacement of Cu by Zn from Cu^{2+} salt solution.
c. Determination of heat of hydration of Na_2SO_4 to Na_2SO_4, 10 H_2O.

7. Distribution law

a. Determination of Composition of Cupric-ammine sulphate formed between $CuSO_4$ and NH_3
b. Determination of equilibrium constant for the reaction $KI+I_2=KI_3$

8. Viscosity and Surface Tension

a. To determine the radius of a molecule from viscosity measurement.
b. To determine the parachor of - CH_2, C and H

I. GENERIC/DISCIPLINE CENTRIC ELECTIVE

INORGANIC CHEMISTRY -II

Course Objectives:

To provide students with the knowledge of inorganic chemistry

CO-1. Alkyls and Aryls of Transition Metal

CO-2. Compounds of Transition Metal-Carbon Multiple Bonds

CO-3. Transition Metal π-Complexes

CO-4. Homogeneous Catalysis

CO-5. Fluxional Organometalilc Compounds

I Alkyls and Aryls of Transition Metals

Types, routes of synthesis, stability and decomposition pathways, organocopper in organic synthesis

II Compounds of Transition Metal-Carbon Multiple Bonds

Alkylidenes, alkylidynes, low valent carbenes and carfaynes- synthesis, nature of bond, structural characteristics, nucleophilic and electrophilic reactions on the ligands, role in organic synthesis

III Transition Metal π-Complexes

Transition metal π-complexes with unsaturated organic molecules, alkenes, alkynes, allyl, diene, dienyl, arene and trienyl complexes, preparations, properties, nature of bonding and structural features. Important reactions relating to nucleophilic and electrophilic attack on ligands and to organic synthesis

IV Transition Metal Compounds with Bonds to Hydrogen

Transition Metal Compounds with Bonds to Hydrogen.

V Homogeneous Catalysis

Stoichiometric reactions for catalysis, homogeneous catalytic hydrogenation, Zeigler-Natta polymerization of olefins, catalytic reactions involving carbon monoxide such as hydrocarbonylation of oletins (oxo reaction), oxopalladation reactions, activation of C-H bond.

VI Fluxional Organometalilc Compounds

Fluxionality and dynamic equilibria in compounds such as h^2- olefin, h^3 allyl and dienyl complexes

Reference Books:

1. Principles and Application of Organotransition Metal Chemistry, J.P. Collman, L.S. Hegsdus, J.R. Norton and R.G. Pinke, University Science Books.
2. The Organometaltic Chemistry o1 the Transition Metals, R.H. Crabtree, John Wiley
3. Metallo-organic Chemistry, A.J. Pearson, Wiley.
4. Organometallic Chemistry, R.C. Mehrotra and A. Singh, New Age International.

Course Outcomes

At the end of this course a candidate will be able to understand –

- Alkyls and Aryls of Transition Metal
- Compounds of Transition Metal-Carbon Multiple Bonds
- Transition Metal π-Complexes
- Homogeneous Catalysis
- Fluxional Organometalilc Compounds

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6	PO-7	PO-8	PO-9	PO-10
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CO-2	3	3	2	1	1	2	2	2	3	2
CO-3	3	2	3	2	2	2	2	2	3	3
CO-4	2	3	3	1	2	2	1	2	2	3
CO-5	3	3	2	2	1	3	2	3	3	3
CO-Average	2.80	2.80	2.40	1.60	1.40	2.40	1.60	2.40	2.80	2.80

3 is strongly mapped , 2 is moderately mapped, 1 is slightly mapped and 0 is non-mapped

II. GENERIC/DISCIPLINE CENTRIC ELECTIVE

INORGANIC CHEMISTRY-III

Course Objectives:

To provide students with the knowledge of inorganic chemistry

CO-1. Metal Storage Transport and Biomineralization

CO-2. Calcium in Biology

CO-3. Metalloenzymes

CO-4. Metals in Medicine

CO-5. Supramolecular Chemistry

I Metal Storage Transport and Biomineralization

Ferritin, transferrin, and siderophores

II Calcium in Biology

Calcium in living cells, transport and regulation, molecular aspects of intramolecular processes, extracellular binding proteins

III Metalloenzymes

Zinc enzymes - carboxypeptidase and carbonic anhydrase. Iron enzymes - catalase, peroxidase and cytochrome P-450. Copper enzymes - superoxide dismutase. Molybdenum oxatransferase enzymes - xanthine oxidase. Coenzyme vitamin BII

IV Metal-Nucleic Acid Interactions

Metal ions and metal complex interactions. Metal complexes - nucieic acids

V Metals in Medicine

Metal deficiency and disease, toxic effects of metals, metals used for diagnosis and chemotherapy with particular reference to anticancer drugs

VI Supramolecular Chemistry

Concepts and language.

(A) Molecular recognition: Molecular receptors for different types of molecules including arisonic substrates, design and synthesis of coreceptor molecules and multiple recognition.

(B) Supramolecular reactivity and catalysis.

(C) Transport processes and carrier design.

(D) Supramolecular devices. Supramolecular photochemistry, supramolecular electronic, ionic and switching devices. Some example of self-assembly in supramolecular chemistry

Reference Books:

1.Principles of Bioinorganic Chemistry, S.J. Lippard and J.M. Berg, University Science Books.
2.Bioinorganic Chemistry, 1. Bertini, H.B. Gray, S.J. Lippard and J.S. Valentine, University Science Books.
3. Inorganic Biochemistry vols I and II. ed. 0.L Eichhom, Elsevier.
4. Progress in inorganic Chemistry, Vols 18 and 38 ed. J.J. Lippard, Wiley.
5. Supramolecular Chemistry, J.M. Lehn, VCH.

Course Outcomes

At the end of this course a candidate will be able to understand –

- Metal Storage Transport and Biomineralization
- Calcium in Biology
- Metalloenzymes
- Metals in Medicine
- Supramolecular Chemistry

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6	PO-7	PO-8	PO-9	PO-10
CO-1	3	3	2	2	2	3	1	3	3	3
CO-2	2	3	2	1	1	2	1	3	2	2
CO-3	2	3	3	1	2	2	3	2	1	2
CO-4	2	2	3	1	1	1	3	1	2	2
CO-5	2	3	2	2	1	3	1	3	1	1
CO-Average	2.20	2.80	2.40	1.40	1.40	2.20	1.80	2.40	1.80	2.00

3 is strongly mapped , 2 is moderately mapped, 1 is slightly mapped and 0 is non-mapped

III. GE/DC PRACTICAL:

PRACTICAL –IV B

INORGANIC CHEMISTRY PRACTICAL

1. Qualitative separation and determination of the following pairs of metal ion using gravimetric and volumetric methods
    a. Ag^{+}(g) and Cu^{2+}(v)
    b. Cu^{2+}(g) and Zn^{2+}(v)
    c. Fe^{3+}(g) and Ca^{2+} (v)
    d. Mg^{2+}(g) and Ca^{2+} (v)

2. Quantitative Analysis
    a. Analysis of alloys (brass, type metal, solder, gun metal) cement, steel using conventional chemical analysis/and physical techniques (if possible).
    (Preferably one alloy and cement analysis may be carried out).

3. Chromatographic Separations

a. Cadmium and zinc
b. Zinc and magnesium.
c. Thin-layer / Paper chromatography-separation of nickel, manganese, cobalt and zinc.Determination of Rf values.

4. Synthesis and characterization of following metal complexes:

a. Sodium tetrathionate Na2S4O6.
b. Metal complex of dimethyl sulfoxide : CuCl2.2DMSO
c. Synthesis of metal acetylacetonate
d. Synthesis of copper and nickel Schiff base complexes.
e. Synthesis of copper and nickel dithiocarbamates
f. $[Co(NH_3)_5\ Cl]\ Cl_2$
g. (ii) $[Co(NH_3)_5\ NO_2]\ Cl_2$
h. (iii)$[Co(NH_3)_5\ ONC]\ Cl_2$

OR,

GENERIC/DISCIPLINE CENTRIC ELECTIVE:

ORGANIC CHEMISTRY -II

Course Objectives:

To provide students with the knowledge of organic chemistry

CO-1. Curve Crossing Model to Chemical Reactions

CO-2. Principals of Reactivity

CO-3. Kinetic Isotope Effect

CO-4. Structural Effects on Reactivity

CO-5. Supramolecular Chemistry

I CurveCrossingModeltoChemicalReactions

Valence bond(VB) configuration mixing diagrams. Relationship between VB configuration mixing and resonance theory. Reaction profiles. Rules for constructing Valance Bond Correlation Diagram. Reactivity pattern based on Valance Bond State Correlation Diagram (VBSCD model). Curve crossing model-nature of activation barrier in chemical reactions.

V.B. Correlation diagram for

One Bond Reactions: V.B. Configuration of Ionic Bond. Heterolysis of Polar Covalent bond in solutions.

Two Bond Process: Covalent Bond: Radical Exchange Reactions, Nucleophilic Exchange Reactions, Nucleophilicity and S_N2 reactivity based on curve- crossing model.

Electrophilic Exchange Reactions. Curve-crossing approach to electrophilic reactivity; Ionic Bond.

II Principals of Reactivity

Mechanistic significance of entropy, enthalpy and Gibb's free energy. Arrhenius equation. Transition state theory. Uses of activation parameters, Hammond's postulate. Bell-Evans Polanyi principle. Potential energy surface model. Marcus theory of electron transfer. Reactivity and selectivity principles.

III Kinetic Isotope Effect

Theory of isotope effects. Primary and secondary kinetic isotope effects. Heavy atom isotope effects, Tunneling effect. Solvent effects.

IV Structural Effects on Reactivity

Linear free energy relationships (LFER).The Hammett equation, substituentS constants, theories ofsubstituent effects. Interpretation of σ-values. Reaction constant ρ. Deviations from Hammett equation. Dual-parameter correlations, inductive substituent constant. The Taft model, σ_L-and σ_R scales.

V Supramolecular Chemistry

Properties of covalent bonds - bond length, inter-bond angles, force constant, bond and molecular dipole moments. Molecular and bond polarizability, bond dissociation enthalpy, entropy.

Intermolecular forces, hydrophobic effects. Electrostatic, induction, dispersion and resonance energy, magnetic interactions, magnitude of interaction energy, forces between macroscopic bodies, medium effects. Hydrogen bond.

Principles of molecular association and organization as exemplified in biological macromolecules like enzymes, nucleic acids, membranes and model systems like micelles and vesicles. Molecular receptors and design principles. Cryptands, cyclophanes, calixeranes, cyclodextrines. Supramolecular reactivity and catalysis. Molecular channels and transport processes. Molecular devices and nanotechnology.

VI Terpenoids and Carotenoids

Classification, nomenclature, occurrence, isolation, general methods of structure determination, isoprene rule. Structure determination, stereochemistry, biosynthesis and synthesis of the following representative molecules: Citral, α-Terpeneol, Zingiberene, Santonin, Bisabolene acid and β-Carotene.

VII Alkaloids

Definition, nomenclature and physiological action, occurrence, isolation, general methods of structure elucidation, degradation, classification based on nitrogen heterocyclic ring, role of alkaloids in plants. Structure, stereochemistry, synthesis and biosynthesis of the following: Ephedrine, (+)-Coniine, Nicotine Atropine, Quinine, Morphine, Narcotine and Reserpine.

VIII Steroids

Occurrence, nomenclature, basic skeleton, Diel's hydrocarbon and stereochemistry. Isolation, structure determination and synthesis of Cholesterol, Bile acids, Androsterone, Testosterone, Estrone, Progestrone, Biosynthesis of steroids

Reference Books:

1. Molecular Mechanics, U. Burkert and N. L. Allinger, ACS Monograph 177, 1982.
2. Organic Chemists' Book of Orbitals. L. Salem and W. L. Jorgensen, Academic Press.
3. Mechanism and Theory in Organic Chemistry, T. H. Lowry and K. C. Richardson, Harper and Row.
4. Introduction to Theoretical Organic Chemistry and Molecular. Modeling, W. B. Smith, VCH, Weinheim.
5. Physical Organic Chemistry, N. S. Isaacs, ELBS/Longman.
6. The Physical Basis of Organic Chemistry, H. Maskill, Oxford University Press.
7. Natural Products: Chemistry and Biological Significance, J.Mann, R.S. Davision, J.B. Hobbs, D.V. Banthrope and J.B. Harborne, Logman, Essex.

Course Outcomes

At the end of this course a candidate will be able to understand –

- CO-1. Curve Crossing Model to Chemical Reactions
- CO-2. Principals of Reactivity
- CO-3. Kinetic Isotope Effect
- CO-4. Structural Effects on Reactivity
- CO-5. Supramolecular Chemistry

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CO-4	2	2	3	1	1	1	3	1	2	3
CO-5	1	3	2	2	1	3	1	3	3	3
CO-Average	2.40	2.20	2.00	1.40	1.60	2.20	1.80	2.20	2.60	2.60

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GENERIC/DISCIPLINE CENTRIC ELECTIVE:

ORGANIC CHEMISTRY-III

Course Objectives:

To provide students with the knowledge of organic chemistry

CO-1. Pericyclic Reactions

CO-2. Heterocycles

CO-3. Synthesis and reactions of pyrylium salts and pyrones

CO-4. Synthesis and reactions of diazines, triazines, tetrazines and thiazines

CO-5. Vitamins

I **Pericyclic Reactions**

Radical stability, polar influences, solvent and steric effects. A curve crossing approach to radical addition, factors effecting barrier heights in additions, regioselectivity in radical reactions, Reactivity, specificity and periselectivity in pericyclic reactions.

Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl system. Classification of periycyclic reactions. Woodward-Hoffmann correlation diagrams. FMO and PMO approach.
Electrocyclic reactions-conrotatory and disrotatory motions, 4n, 4n+2 and allyl systems. Cycloadditions-antarafacial and suprafacial additions, 4n and 4n+2 systems. 2+2 addition of ketenes, 1,3 dipolar cycloadditions and cheleotropic reactions.

Sigmatropic rearrangements-suprafacial and antarafacial shifts of H, sigmatropic involving carbon moieties, 3,3- and 5,5- sigmatropic rearrangements. Claisen, Cope and aza-Cope rearrangements. Fluxional tautomerism. Ene reaction.

II **Heterocycles:**

Nomenclature & Classification

Replacement and systematic nomenclature (Hantzs MCH-Widman system) for monocyclic fused and bridged heterocycles.

AromaticHeterocycles

Criteria of aromaticity including ring current and chemical shifts in 1H NMR spectra.

Non-aromaticHeterocycles

Conformation of six-membered heterocycles with reference to molecular geometry, barrier to ring inversion, pyramidal inversion and 1,3-diaxial interaction.

Heterocyclic Synthesis: Princples of heterocyclic synthesis involing cyclization reactions and cycloaddition reactions.

III **Small ring Heterocycles**

Three, Four & Five membered heterocycles including medicinal applications of benzopyrroles, benzofurans and benzothiophenes

IV **Six-Membered Heterocycles with one Heteroatom**

Synthesis and reactions of pyrylium salts and pyrones and their comparison with pyridiniurn & thiopyrylium salts and pyridones. Synthesis and reactions of quinolizinium and benzopyryliumsalts, coumarins and chromones.

V Six-Membered Heterocycles with Two or More Heteroatoms

Synthesis and reactions of diazines, triazines, tetrazines and thiazines

VI Seven- and Large-Membered Heterocycles

Synthesis and reactions of azepines, diazepines.

VII Heterocyclic Systems Containing P, As, Sb & B

Heterocyclic rings containing phosphorus: introduction, nomenclature, Synthesis and characteristics of 5- and 6-membered ring systems-phosphorinanes, phosphorines, phospholanes and phospholes.

Heterocyclic rings containing As and Sb: Introduction, synthesis and characteristics of 5- and 6-membered ring systems.

Heterocyclic rings containing B: Introduction, synthesis reactivity and spectral characteristics of 3- 5- and 6- membered ring system.

VIII Vitamins

Determination and Synthesis of Vit. A, B,, B_Z, B_6, Vit. C and Vit. D.

Reference Books:

1. Pericyclic Reactions, S.M. Mukherji, Macmillan, India.
2. Molecular Mechanics, U. Burkert and N.L. Allinger, ACS Monograph 177, 1982.
3. Organic Chemists' Book of Orbitals. L. Salem and W.L. Jorgensen, Academic Press.
4. Mechanism and Theory in Organic Chemistry, T.H. Lowry and K.C. Richardson, Haper and Row.
5. Supramolecular Chemisrty, Concepts and Perspectives, J.M. Lehn, VCH.
6. Heterocyclic Chemistry Vol. 1-3, R. R. Supta, M. Kumar and V Gupta, Springer Verlag.
7. Heterocyclic Chemistry. T.L Gilchrisl. Longman Scietific Teehinai.
8. Natural Produds; Chemistry and Biological Significance, J. Mann, R. S. Davidson, J.B. Hobbs, D.V, Banthirope and J. B. Harbome, Longman,Essex.
9. Organic Chemistry, Vol 2, l. L. Finar, ELB S.
10. Stereoselective Synthesis; A Practical Approach, M. Nogradi. VCH.
11. Chemistry, Biological and Pharmacological Properties of Medicinal lants from the Americas, Ed. Kurt Hosiettmann, M. P. Gupla and A. Marston, Harwood Academic Publishers.

Course Outcomes

At the end of this course a candidate will be able to understand –

- Pericyclic Reactions
- Heterocycles
- Synthesis and reactions of pyrylium salts and pyrones
- Synthesis and reactions of diazines, triazines, tetrazines and thiazines
- Vitamins

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CO-3	2	2	1	2	2	1	3	2	3	2
CO-4	3	3	3	1	1	1	1	3	2	1
CO-5	3	3	1	2	1	3	1	3	3	3
CO-Average	2.80	2.80	1.80	1.60	1.60	1.80	1.80	2.60	2.80	2.00

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GE/DC PRACTICAL:

PRACTICAL –IV C

ORGANIC CHEMISTRY PRACTICAL

1. **Characterization of organic compounds**

   It is expected to carry out separation, purification and identification of the components of a mixture of three organic compounds (three solids or two liquids and on solid, two solids and one liquid). Student should also check the purity of the separated components on TLC plates.

2. **Extraction of Organic compounds from Natural Sources**
   a. Isolation of Caffeine from Tea Leaves (Ref. Experimental Organic Chemistry H Dupon Durst. George W.Gokel, p.464 McGraw Hall Book Co., New York).
   b. Isolation of Casein from milk (Some typical colour reactions of proteins).
   c. Isolation of lactose from milk (purity of sugar should be checked by LC and PC and Rfvalues reported).
   d. Isolation of Nicotine dipicrate from tobacco
   e. Isolation of piperine from black pepper
   f. Isolation of Lycopene from tomatoes
   g. Isolation of β-carotene from carrots
   h. Isolation of Oleic acid from olive oil
   i. Isolation of Eugenol from cloves
   j. Isolation of (+)Limonine from citrus rinds

3. **Multistep Synthesis of Organic Compounds**

   The exercise should illustrate the use of organic reagents and may involve purification of the products by chromatographic techniques.
   a. Beckman rearrangement: Benzanilide from benzene
      Benzene → Benzophenone → Benzophenone oxime →Benzanilide
   b. Benzilic acid rearrangement: Benzilic acid from benzoin
      Benzoin → Benzil → Benzilic acid
   c. Synthesis using microwaves
      Alkylation of diethyl malonate with benzyl chloride
   d. Synthesis using phase transfer catalyst
      Alkylation of diethyl malonate or ethyl acetoacetate with an alkyl halide

4. **Some illustrative exercises are given below**:
    a. Estimation of phenol / aniline using bromate bromide solution/or acetylation method
    b. Estimation of carbonyl group by using 2,4-dinitrophenyl hydrazine
    c. To determine the percentage or number of phenolic groups in the given sample by the acetylation method.

5. **Identification of organic compounds**
   By the analysis of their spectral data (UV, IR PMR, CMR & MS).

6. **Spectrophotometric (UV/VIS) Estimations**
    a. Amino acids
    b. Proteins
    c. Carbohydrates
    d. Cholesterol
    e. Ascorbic acid
    f. Aspirin
    g. Caffeine

IV. CORE COURSE (PROJECT):

PROJECT WORK

Each student has to submit the dissertation work duly forwarded by the HOD of Department concerned.

Head
Department of Chemistry
Netaji Subhas University

NETAJI SUBHAS UNIVERSITY Jamshedpur

Dean Academics
Netaji Subhas University
Jamshedpur, Jharkhand