

**SAKTHI COLLEGE OF ARTS AND SCIENCE FOR WOMEN, ODDANCHATRAM**

**(Recognized Under Section 2(f) and 12(B) of UGC Act 1956)**

**(Affiliated to Mother Teresa Women's University, Kodaikanal)**

**PG AND RESEARCH DEPARTMENT OF CHEMISTRY**

**CURRICULUM FRAMEWORK AND  
SYLLABUS FOR OUTCOME BASED EDUCATION IN**

**M.Sc., CHEMISTRY**

**FRAMED BY**

**MOTHER TERESA WOMEN'S UNIVERSITY, KODAIKANAL**

**UNDER**

**CHOICE BASED CREDIT SYSTEM**

**2018 - 2021**

**PREAMBLE:**

The objective of any programme at Higher Education Institute is to prepare their students for the society at large. Sakthi College of Arts and Science envisions all its programmes in the best interest of its students. With this vision, the Department of Chemistry has been incepted with the introduction of B.Sc., (Chemistry) in 2009. Comprehending the need of its learners for higher studies, the institution introduced M.Sc., (Chemistry) in 2010 and M.Phil., (Chemistry) in 2014.

M.Sc., (Chemistry) is a post graduation course, which will allow the students to develop in depth understanding of various aspects of the subject. The conceptual understanding, development of experimental skills, designing and implementation of novel synthetic methods, developing the aptitude for academic and professional skills, acquiring basic concepts for structural elucidation with hyphenated techniques, understanding the fundamental biological processes and rationale towards computer assisted drug designing are among such important aspects.

**Fixing the Learning Objectives:**

Since the Academic year 2018 – 2019, the learning objectives and outcomes of the programmes B.Sc., (Chemistry), M.Sc., (Chemistry) and M.Phil., (Chemistry) have been set, following the Bloom's Taxonomy Cognitive Domain. Accordingly, it is broken into six levels of learning objectives of each course. They are -

K1 / Knowledge = Remember

K2 / Comprehension = Understand

K3 / Application = Apply

K4 / Analysis = Analyze

K5 / Evaluation = Evaluate

K6 / Synthesis = Create

**Mapping COs with POs:**

For each programme, the Educational objectives and the Specific objectives are specified. The programme outcomes are designed according to the curriculum, teaching, learning and evaluation process. For each course, the definite outcomes are set, giving challenge to the cognitive domain. The course outcomes are mapped with the programme outcomes. The performance of the stakeholders is assessed and the attainment rate is fixed, by using the measurements 'high', 'medium' and 'low'. The restructuring of the curriculum is done based on the rate of attainment.

**Institutional Objectives:**

The institution has certain definite Institutional Objectives to be attained.

- Skill Development & Capacity Building
- Women Empowerment
- Self-reliance
- Gender Equity & Integrity

### Programme Specific Objectives:

The Post Graduates of M.Sc. Chemistry Programme will be able to

- **PEO1:** Apply chemical principles and theories and acquire skills in synthesis, instrumentation and characterization.
- **PEO2:** Apply laboratory skills and critical thinking to develop applications for solving Industry oriented problems.
- **PEO3:** Function as a team member and develop projects in a multi-disciplinary environment by emulating leadership skills.
- **PEO4:** Work productively as chemistry professional by adopting to environment with lifelong learning and adhering to ethical standards and apply the knowledge acquired for the improvement of the society.

### Mapping PEOs with IOs:

Programme Educational Objectives	Institutional Objectives			
	1	2	3	4
<b>B.Sc., M.Sc., and M.Phil., (Chemistry)</b>				
<b>PEO1:</b> Applying chemical principles and theories and acquire skills in synthesis, instrumentation and characterization.	*			
<b>PEO2:</b> Applying laboratory skills and critical thinking to develop applications for solving Industry oriented problems.		*		
<b>PEO3:</b> Functioning as a team member and develop projects in a multi-disciplinary environment by emulating leadership skills.			*	
<b>PEO4:</b> Working productively as chemistry professional by adopting to environment with lifelong learning and adhering to ethical standards and apply the knowledge acquired for the improvement of the society.				*

**Measuring: H – High; M – Medium; L – Low**

## M.Sc., CHEMISTRY

### Programme Outcomes:

- PO1:** Understanding the application of the classical subjects in modern Chemistry and master factual and experimental knowledge across the principal areas of Chemistry
- PO2:** Demonstrating competence in solving industrial scientific problems through experimental, computational and/or data analysis models
- PO3:** Involving in deeper learning of the principles of Organic, Inorganic and Physical Chemistry
- PO4:** Learning modern analytical and spectroscopic tools and their applications to different disciplines of Chemistry
- PO5:** Designing and conducting experiments as well as to analyze and interpret the data
- PO6:** Learning the interdisciplinary nature of chemistry and to integrate the knowledge with a variety of chemical problems
- PO7:** Learning, designing and demonstrating sustainable industrial reactions within realistic constraints such as economic, environmental, social, ethical, health, safety and productivity

**ASSESSMENT PATTERN**  
**CIA / QUESTION PATTERN & SCHEME**

S.No	Section	Question Type	Marks Allotted
1	Part - A	Six questions in multiple choice pattern, testing K1 and K2 are to be given. Each question carries one mark.	03X01 = 03
2	Part - B	Two descriptive questions, with alternate options, testing K3 and K4, are to be given. Each question carries four marks.	02X02 = 04
3	Part - C	Two descriptive questions, testing K5 and K6, are to be given. Three questions are to be answered. Each question carries 15 marks.	02X04 = 08
4		Assignment	05
5		Seminar	05
Total Marks in CIA			25

**CE / QUESTION PATTERN & SCHEME**

S.No	Section	Question Type	Marks Allotted
1	Part - A	Ten questions in multiple choice pattern, testing K1 and K2 are to be given. From each unit, two questions must be taken. Each question carries one mark.	10X1 = 10
2	Part - B	Five descriptive questions, with alternate options, testing K3 and K4, are to be given. Each question carries four marks. Questions are taken in the given order. Qtn. No. 11 (a) or (b) from Unit I Qtn. No.12 (a) or (b) from Unit II Qtn. No.13 (a) or (b) from Unit III Qtn. No.14 (a) or (b) from Unit IV Qtn. No.15 (a) or (b) from Unit V	5X4 = 20
3	Part - C	Six descriptive questions, testing K5 and K6, are to be given. Three questions are to be answered. Each question carries 15 marks. Questions are taken in the given order. Qtn. No. 16 from Unit I Qtn. No. 17 from Unit II Qtn. No. 18 from Unit III Qtn. No. 19 from Unit IV Qtn. No. 20 from Unit V	3X15 = 45
Total Marks in CE			75

**COMMON ACADEMIC STRUCTURE / M.Sc., (CHEMISTRY) / 2018 – 2021**

Sem	Sub. Code	Title of the Course	Hr s	Credits	Marks		
					CIA	CE	Total
I	PCHT11	Part – III / Core – I / Organic Chemistry I	5	5	25	75	100
	PCHT12	Part – III / Core – II / Inorganic Chemistry I	5	5	25	75	100
	PCHT13	Part – III / Core – III / Physical Chemistry I	5	5	25	75	100
	PCHP11	Part – III / Core Practical – I / Organic Chemistry	5	5	25	75	100
	PCHE11	Part – III / Elective-I / Medicinal Chemistry (or) Drug Design	5	5	25	75	100
		<b>Total</b>		<b>25</b>	<b>25</b>		
II	PCHT21	Part – III / Core – IV / Organic Chemistry II	5	5	25	75	100
	PCHT22	Part – III / Core – V / Inorganic Chemistry II	5	5	25	75	100
	PCHT23	Part – III / Core – VI / Physical Chemistry II	5	5	25	75	100
	PCHP22	Part – III / Core Practical – II / Inorganic Chemistry	5	5	25	75	100
	PCHE22	Part – III / Elective-II / Analytical Techniques	5	5	25	75	100
		<b>Total</b>		<b>25</b>	<b>25</b>		
III	PCHT31	Part – III / Core – VII / Organic Chemistry III	5	5	25	75	100
	PCHT32	Part – III / Core – VIII / Inorganic Chemistry III	5	5	25	75	100
	PCHT33	Part – III / Core – IX / Physical Chemistry III	5	5	25	75	100
	PCHP33	Part – III / Core Practical – II / Physical Chemistry	5	5	25	75	100
	PCHE33	Part – III / Elective-III / Environmental Chemistry (or) Green Chemistry	5	5	25	75	100
		<b>Total</b>		<b>25</b>	<b>25</b>		
IV	PCHT41	Part – III / Core – X / Chemistry of Natural Products and Bioinorganic Chemistry	5	5	25	75	100
	PCHT42	Part – III / Core – XI / Nano-Chemistry and Super-molecular Chemistry	5	5	25	75	100
	PCHP43	Project work	5	5	40	60	100
		<b>Total</b>		<b>15</b>	<b>15</b>		
<b>Grand Total</b>			<b>90</b>	<b>90</b>			<b>1800</b>

**Programme: M.Sc.,**

**Semester: I**

**Course Type: Core Paper-I**

**Hours Required: 5 Hrs / Week**

**CA: 75**

**Subject: Chemistry**

**Course: Organic Chemistry I**

**Credits:5**

**CIA: 25**

**Course Outcomes:**

After completion of the course, certain outcomes are expected from the learners.

Description of COs	Bloom's Taxonomy Level
Identifying the different types of reactive intermediates and appreciating their importance in organic reactions	Application (Level 3)
Identifying aromatic, non-aromatic and anti-aromatic compounds	Knowledge (Level 1)
Understanding the various mechanisms of organic reactions	Comprehension (Level 2)
Understanding and apply the concepts of stereochemistry	Comprehension (Level 2)
Appreciating the importance of different types of reactive intermediates in organic reactions.	Synthesis (Level 6)

**COURSE CONTENT**

**Unit I Reactive intermediates and Aromaticity**

Carbocations, carbanions, carbenes, benzyne and nitrenes - Generation, stability and reactivity. Aromatic character: Six-, five-, seven-, and eight- membered rings - Other systems with aromatic sextets – Huckel's theory of aromaticity, concept of homoaromaticity and antiaromaticity, Electron occupancy in MO's and aromaticity - NMR concept of aromaticity and antiaromaticity, systems with 2,4,8 and 10 electrons, systems with more than 10 electrons, alternant and non-alternant hydrocarbons (azulene type). Bonding properties of systems with  $(4n+2)\pi$  electrons and  $4n\pi$  electrons, Heteroaromatic molecules. Annulenes, heteroannulenes, sydnones and fullerenes. Craig's rule, Hammond's postulate

**Unit II Substitution reactions**

**Nucleophilic Substitution**

1. Aliphatic nucleophilic substitution:  $S_N1$  and  $S_N2$  mechanism – Kinetic and stereochemical characteristics – effects of substrate structure, nature of the nucleophile and leaving group on the rate – solvent effects – examples of  $S_Ni$  substitution – Neighbouring group participation-Anchimeric assistance
2. Aromatic nucleophilic substitution: Benzyne and Meisenheimer intermediates

**Electrophilic Substitution**

1. Mechanism of aliphatic electrophilic substitution reaction –  $S_E1$ ,  $S_E2$ ,  $S_{EI}$  reaction.
2. Mechanism of aromatic electrophilic substitution reactions – complexes – nitration,

halogenation, sulphonation, Friedel Craft alkylation and acylation – Reimer Tiemann reaction. Linear free energy relationship – Hammett equation – Significance of the  $\sigma$  and  $\rho$  parameters; Taft equation.

### **Unit III Addition and Elimination reactions**

#### **Addition reactions**

Regio and stereochemistry of addition of halogens and halogens acids to carbon – carbon multiple bonds – hydroboration – addition to carbonyl bonds – mechanism of Aldol, Perkin, Stobbe, Dieckmann condensation, Reformatsky and Grignard reaction, Michael addition reaction and Mannich reaction – Formation and Synthetic application of enamines – Stork enamine reaction.

#### **Elimination reactions**

E1, E2, E1CB mechanism – structural and solvent effect on these mechanisms – orientation of double bonds (regio and stereoselectivities) – competition between substitution and elimination reaction – cis elimination, pyrolytic eliminations

### **Unit IV Rearrangements**

Definition – nucleophilic, electrophilic and free radical rearrangements – intramolecular and intermolecular rearrangements – migratory aptitude – Wagner – Meerwin, Benzil – Benzilic acid, Schmidt, Lossen, Curtius, Beckmann, Fries, Baeyer Vileger, Favorski, Stevens and Neber rearrangements.

### **Unit V Introduction to stereochemistry**

Concept of chirality: specification on configuration by Cahn, Ingold and Prelog system of notation, compounds with more than one chiral centre – calculation of number of stereoisomers – erythro and threo nomenclature; interconversions of Sawhorse, Fisher and Newman's Projections.

The concept of prochirality: Topicity and prostereoisomerism – equivalent, enantiotopic and diastereotopic ligands and faces. Atropisomerism – concept of axial chirality „R“ and „S“ nomenclature of some axially chiral molecules.

Geometrical isomers – E & Z nomenclature determination of configuration of geometrical isomers by physical and chemical methods.

#### **Books for study**

1. E.L.Eliel, Stereochemistry of Carbon Compounds, McGraw Hill, 1962.
2. V.M.Potapov, Stereochemistry, MIR Publishers, Moscow 1979.
3. D.Nasipuri, Stereochemistry of Organic compounds, 2<sup>nd</sup> Edn, New Age International, New Delhi, 1972.

### **Books for reference**

1. E.L.Eliel , N.C.Allinger, S.J.Angyal and G.A.Morrison, Conformational analysis, Interscience, New York, 1965.
- 2.C.Djerassi, Optical Rotatory Dispersion – Application to Organic Chemistry, McGraw Hall, 1960.
- 3.R.E.Ireland, Organic Synthesis, Prentice Hall, 1969.
- 4.S.Turner, Design of Organic Synthesis, Elsevier, 1976

### **Online Resource**

- 1.[https:// www.teacheron.com/online-organic chemistry-tutors](https://www.teacheron.com/online-organic-chemistry-tutors)
- 2.<https://www.masterorganicchemistry.com/>

**Programme: M.Sc.,**

**Subject: Chemistry**

**Semester: I**

**Course: Inorganic Chemistry I**

**Course Type: core Paper I**

**Credits: 5**

**Hours Required: 5 Hrs / Week**

**CIA : 25 / CA:75**

**Course Outcomes:**

After completion of the course, certain outcomes are expected from the learners.

<b>Description of COs</b>	<b>Bloom's Taxonomy Level</b>
Predicting the Chemistry theories involved and structure of ionic compounds	Comprehension (Level 2)
Assessing the types of hybridization involved in ionic solids	Evaluation (Level 5)
Identifying the type of crystal structure exist in ionic solids	Comprehension (Level 2)
Describing the type of defects in metals, and solid state reaction	Evaluation (Level 5)
Applying different electron counting rules to predict the shape/geometry of Interhalogens and polymeric Inorganic compounds	Application (Level 3)

**COURSE CONTENT**

**Unit I Covalent Bonding**

V.B. approach to bonding-Hitler-London, Pauling and Slater refinements, Concept of hybridization and structure of molecules, VSEPR theory shapes of molecules. M.O. approach to covalent bonding – symmetry and overlap of atomic orbitals – symmetry of molecular orbitals – sigma, pi and delta bondings – energy levels in homo and hetero nuclear diatomic systems – bond length, bond order and bond energy, Application to small molecules such as  $\text{BeCl}_2$ ,  $\text{BCl}_3$  and  $\text{CCl}_4$ ,  $\text{SF}_4$ , ionic character in a covalent bond. The concept of multicentre bonding.

**Unit II Metallic Bonding**

Drude Lorentz theorem, merits and demerits – Sommerfield theorem – band theorem– formation of Brillion Zones – conductors and insulators and semiconductors, – Hall effect – super conductors, photoconductivity. Point-, line- and plane defects in solids – Stoichiometric and non-stoichiometric defects – Frenkel and Schottky defects. Effect of imperfections on physical properties like electrical conductivity, thermal, optical and magnetic phenomena.

**Unit III Solid State – Structure**

Cohesive energy and Madelung constants, Van der Waals forces, Close packing of atoms and ions HCP and BCC types of packing voids, radius ratio – derivation – its influence on structures. Lattice energy – Born-Landé equation - Kapustinski equation. Representative structures of AB and  $\text{AB}_2$  types of compounds - rock salt, cesium chloride, wurtzite, zinc

blende, rutile, fluorite, antiferite, cadmium iodide and nickel arsenide. Structure of graphite and diamond. Spinel - normal and inverse types and perovskite structure

#### **Unit IV Main Group Chemistry**

Chemistry of boron – borane, higher boranes, carboranes, borazines and boron nitrides. Chemistry of silicon – silanes, higher silanes, multiple bonded systems, silicon nitrides, siloxanes. P-N compounds, cyclophosphazenes and cyclophosphazanes. S-N compounds –  $S_4N_4$ ,  $(SN)_x$ .

#### **Unit V Interhalogens and Polymeric Inorganic Compounds**

Pseudo halogens; , Structure and bonding in  $ClF_3$ ,  $BrF_3$  ,  $BrF_5$  ,  $IF_5$ ,  $IF_7$  etc . Oxides and oxoacids of halogens, Isopoly and heteropoly acids – Structure and bonding of 6- and 12 – isopoly and heteropoly anions. Structure of silicates - applications of Paulings rule of electrovalence - isomorphous replacements in silicates – ortho, meta and pyro silicates – one dimensional, two dimensional and three dimensional silicates – Bonding in Noble gas compounds –  $XeCl_2$ ,  $XeF_4$ ,  $XeOF_4$ ,  $XeF_6$ .,

#### **Books for study:**

1. J.E. Huheey, Inorganic Chemistry, 3<sup>rd</sup> Ed., Harper & Row publisher, 1983.
2. J.D. Lee, Concise Inorganic Chemistry, 5<sup>th</sup> Ed, Wiley, 1999.
3. William Jolly, Advanced Inorganic Chemistry

#### **Books for reference:**

1. D.E. Douglas, D.H. McDaniel, J.J. Alexander, Concepts and Models in Inorganic Chemistry, 3<sup>rd</sup> Ed. 1994.
2. M.C. Day, J. Selbin, Theoretical Inorganic Chemistry, 2<sup>nd</sup> Ed., East West Press, 1985.
3. F. Basolo, R.G. Pearson, Mechanism of Inorganic Reactions, 2<sup>nd</sup> Ed., John Wiley, 1967.
4. L. Pauling, The Nature of the Chemical Bond, 3<sup>rd</sup> Ed., Cornell University Press, 1960.
5. F.A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry, 4<sup>th</sup> Ed., John Wiley & Sons, 1986

#### **Online Resource:**

1. <https://tutorme.com/inorganic-chemistry-tutors/>
2. [https://chem.libretexts.org/Bookshelves/Inorganic\\_Chemistry](https://chem.libretexts.org/Bookshelves/Inorganic_Chemistry)

**Programme:** M.Sc.,

**Subject:** Chemistry

**Semester:** I

**Course:** Physical Chemistry I

**Course Type:** Core Paper I

**Credits:** 5

**Hours Required:** 5 Hrs/week

**CIA:** 25 /CA:75

**Course Outcomes:**

After completion of the course, certain outcomes are expected from the learners.

Description of COs	Bloom's Taxonomy Level
Deriving the concept of Gibb's duhem rule, Nernst equation, laws of thermodynamics	Creation (Level 6)
Understanding the concept of distribution and chemical kinetics, uses of Hammet equation.	Understanding (Level 2)
Evaluating most probable distribution state for all type of statistics i.e. for Maxwell Boltzmann, Fermi dirac and Bose –Einstein statistics.	Evaluation (Level 5)
Analyzing the concept of strong and weak electrolyte, Debye Huckel rules.	Analysis (Level 4)
Applying the concepts of photochemistry and laws	Application (Level 3)

**COURSE CONTENT**

**Unit I** Thermodynamics Chemical and Phase Equilibrium

The second law of thermodynamics – Entropy – thermodynamics of systems of variable compositions – partial molar quantities and their determination – chemical potential – Gibbs-Duhem equation – Activity and Fugacity- determination of fugacity, Nernst equation, Third law of thermodynamics, exceptions and applications. Chemical equilibrium - temperature dependence, Vant-Hoff equation, Non-equilibrium thermodynamics - postulates and methodology. Phase equilibrium-Application to three component system- $\text{CH}_3\text{COOH}$ ,  $\text{H}_2\text{O}$  and  $\text{CHCl}_3$  system.

**Unit II** Chemical Kinetics

Derivation of rate constant for opposing, consecutive and parallel reaction-steady state approximation. Chain reactions: kinetics of decomposition of  $\text{N}_2\text{O}_5$  – Non stationary chain reaction:  $\text{H}_2\text{O}_2$  reaction and explosion limits. Grunwald –Winstein equation on reaction rates. Concept of Linear Free Energy Relationships-derivation of Hammett equation-significance of substituent and reaction rate constants - Taft equation - thermodynamic implications of LFER. Experimental methods for the study of fast reaction-flow method-relaxation methods.

**Unit III** Electrochemistry – I

Mean ion activity and activity coefficient of electrolytes in solution – Ion association - Ionic strength – Debye-Huckel theory – Debye-Huckel limiting law - its validity and limitations – Strong and weak electrolytes – Debye theory of electrolytic conductance – Debye – Huckel – Onsager equation - Verification and limitations - Electrochemical cells and applications of standard potentials. Batteries-Primary and secondary fuel cells – Corrosion and corrosion inhibition

#### **Unit IV Electrochemistry – II**

The electrical double layer – Polarizable and non-polarizable interfaces – Structure of electrical double layer – Electrocapillary and double layer capacity measurements – Double layer models – Helmholtz, Guoy–Chapman and Stern models.

Electrokinetic phenomena: Zeta potential – Electrophoresis Electroosmosis, sedimentation potential and streaming potential, Kinetics of electrode processes – Current– potential curve – Butler–Volmer relation and its approximations – Tafel equation – Charge transfer resistance – Nernst equation from Butler–Volmer equation –Multistep processes – Symmetry factor and transfer coefficient – Electrocatalysis–Hydrogen evolution reaction as a case study.

#### **Unit V Photochemistry**

Absorption of light by molecules, reaction paths of electronically excited molecules – de-excitation pathways, Fluorescence and Phosphorescence – Jablanski diagram – Physical properties of the electronic excited molecules – excited state dipole moments, excited state pKa and redox potentials – Stern – Volmer equation and its application – photosensitization – Chemi Luminescence – Quantum Yield and actinometry.

#### **Books for study**

1. P.W. Atkins, Physical Chemistry, 7<sup>th</sup> Ed., Oxford University press, 2002.
2. J. Rajaram and J.C. Kuriacose, 2<sup>nd</sup> Ed., Thermodynamics for Students of Chemistry – Classical, Statistical and Irreversible, Shobhan Lal Nagin, New Delhi, 1996.
3. G.W.Castellan, Physical Chemistry, Narosa, 1996.
4. K.J. Laidler, Chemical Kinetics, 3<sup>rd</sup> Ed., Pearson Education, 2004.
5. S. Glasstone, Text book of Physical Chemistry, McMillan, 1974.
6. K.K. Rohatgi – Mukherjee, Fundamentals of Photochemistry, New Age International, 2000.

#### **Books for reference**

1. J. Moore, Physical Chemistry, 5<sup>th</sup> Edn., Orient Longman.1972
2. S. Glasstone, Thermodynamics for Chemists, Affiliated East West Press, 1969.
3. I.M. Klotz, P.M. Rosenberg, Chemical Thermodynamics: Basic Concepts and

Methods, 7<sup>th</sup> Ed., John Wiles & Sons, 2008.

4. A.A. Frost, R.G.Pearson, Kinetics and Mechanism, John Wiley & Sons, 1953.

**Online Resource:**

1. <https://www.khanacademy.org>
2. <https://www.varsitytutors.com>
3. <https://www.coursera.org>

**Programme: M.Sc.,**

**Subject: Chemistry**

**Semester: I**

**Course: Organic Chemistry**

**Course Type: Core Practical -I**

**Credits:5**

**Hours Required: 5 Hrs / Week**

**CIA:25/CA:75**

**Course Outcomes:**

After completion of the course, certain outcomes are expected from the learners.

<b>Description of COs</b>	<b>Bloom's Taxonomy Level</b>
Learning simple extraction techniques	Knowledge (Level 1)
Understanding basic chromatographic methods.	Comprehension (Level 2)
Understanding and develop the principles of quantitative and qualitative analysis of organic compounds.	Comprehension (Level 2)
Developing skill in simple organic synthesis	Synthesis (Level 6)
Developing the principles of quantitative and qualitative analysis of organic compounds.	Synthesis (Level 6)

### **COURSE CONTENT**

1. Purification techniques of organic compounds and their spectroscopic identifications.
  - a) Purification of binary mixtures by Thin Layer Chromatography (TLC) and Column chromatography
  - b) Purification of tertiary mixture of amino acids by paper chromatography  
(Both experiments demonstration only)
2. Extraction of natural products such as Caffeine, Caesin.
3. Organic preparation : Any 4 preparations (involving two or more than two steps) involving the following representative reactions-
  - 1) Bromination
  - 2) Hydrolysis
  - 3) Nitration
  - 4) Condensation
  - 5) Oxidation
4. Qualitative analysis – Separation of two component mixture and identification of components by chemical methods (about 4 – 5 mixtures)
5. Quantitative Analysis
  - a) Estimation of ascorbic acid
  - b) Estimation of glucose

**Books for study**

1. Ahluwalia V. K Comprehensive Practical Organic Chemistry

**Books for reference**

1.vogel practical organic chemistry

**Online resource**

1.<http://rushim.ru/books/praktikum/Mann.pdf>

Programme: M.Sc.,

Subject: Chemistry

Semester: I

Course: Medicinal Chemistry and Drug Design

Course Type: Part – III / Elective-I

Credits: 5

Hours Required: 5Hrs / Week

CIA:25 / CA:75

### Course Outcomes:

After completion of the course, certain outcomes are expected from the learners.

Description of COs	Bloom's Taxonomy Level
Analyzing the effect of different drugs	Analysis (Level 4)
Describing the mechanism of different DFT	Understanding (Level 2)
Finding drugs present in different Pharmaceutical compounds	Analysis (Level 4)
Applying the concept of molecular modeling and drug design in research fields.	Application (Level 3)
Designing the bio-inorganic compounds in medicine in future research work.	Creation (Level 6)

## COURSE CONTENT

### Unit I Molecular modeling and Computer aided drug design.

Basic features of molecular modeling-Simulation for conformational analysis;Molecular mechanics, *Ab initio*, DFT and semi-empirical methods-Energy minimization; Local and global energy minima, saddle point-Electronic descriptors-Force fields-Monto Carlo t

Molecular docking- Molecular Dynamics; Introduction, basic principles, conformation analysis, Mechanics and dynamics of Bio-macromolecules.

Stages in drug development-conventional approach-Rational drug design-Target identification-Sequence to structure - Protein structure prediction - Homology modeling- Active sites-Lead structure identification, Target – Substrate Docking - Scoring-molecular descriptors - High throughout screening and combinatorial chemistry-Structure-activity relationship (SAR)– Toxicity, Patents

### Unit II Medicinal Bioinorganic Chemistry

Bioinorganic Chemistry of quintessentially toxic metals. Lead, Cadmium, Mercury, Aluminum, Chromium, Iron, Copper, Plutonium. Detoxification by metal chelation. Drugs that act by binding at the metal sites of Metalloenzymes.

Chemotherapy-Chemotherapy with compounds of certain non-essential elements. Platinum complexes in Cancer therapy – Cisplatin and its mode of action – Cytotoxic compounds of other metals – Gold containing drugs as anti-rheumatic agents and their mode of action - Lithium in Pschycopharmacological drugs. Molecular channels and transport processes.

### **Unit III Medicinal Bioorganic Chemistry**

Introduction – Study of drugs – Important terminologies in pharmaceutical chemistry – Classification and nomenclature of drugs – Antibacterial drugs – Sulpha drugs: sulphanilamide, sulphadiazine –

Antibiotics: chlorphenicol, penicillin, Analgesics: morphine, heroin – Anticonvulsant: Barbiturates, oxazolindiones, streptomycin, terramycin

### **Unit IV Vitamins**

Vitamins A, B<sub>1</sub>, B<sub>2</sub>, C, E and H

### **Unit V Drug Action**

Mechanism of action of drugs – Metabolism of drugs – Absorption of drugs, Diabetes: control of diabetes, insulin – Cancer and antineoplastic drugs: antimetabolites, plant products – Cardio vascular drugs: Antiarrhythmic drugs, antihypertension drugs

### **Books for study**

1. Andrew Leach, Molecular Modelling, Principles and Applications, 2<sup>nd</sup> Ed., Pearson, Prentice Hall, 1991.
2. G.L. Patrick, An Introduction to Medicinal Chemistry, Oxford University, Press, 2<sup>nd</sup> Ed., 2001.
3. A. R Leach, V. J. Gillet, An Introduction to Cheminformatics, Springer, The Netherlands, 2007.

### **Books for reference**

1. J. Ghosh, Fundamental Concepts of Applied Chemistry, S. Chand and Co., New Delhi, 2006.
2. G. Thomas, Fundamentals of Medicinal Chemistry, John Wiley & Sons, 2003
3. A. Burger, Medicinal chemistry, I arts I and II, Wiley, N. Y., 1969.

### **Online resource**

1. <http://www.blinkprods.com>
2. <https://www.intechopen.com/books/drug->
3. <https://www.omicsonline.org>

**Programme: M.Sc.,**

**Semester: I**

**Course Type: Core Paper-I**

**Hours Required: 5 Hrs / Week**

**Subject: Chemistry**

**Course: Organic Chemistry II**

**Credits: 5**

**CIA : 25 / CA:75**

**Course Outcomes:**

After completion of the course, certain outcomes are expected from the learners.

<b>Description of COs</b>	<b>Bloom's Taxonomy Level</b>
Gaining knowledge and understanding of the various reagents in organic synthesis and important oxidation and reduction reactions.	Knowledge (Level 1)
Understanding and applying the various reagents in organic synthesis and design organic synthetic reactions.	Understanding (Level 2)
Evaluating the stability of various conformers of acyclic and cyclic systems using steric, electronic and stereoelectronic effects and correlate them to reactivity.	Evaluation (Level 5)
Applying asymmetric transformations in a logical manner for the synthesis of chiral molecules	Application (Level 3)
Using various models for determining stereo selectivity of various organic transformation	Synthesis (Level 6)

**COURSE CONTENT**

**Unit I** Conformational analysis of acyclic and cyclic system

Definition – restricted rotation about carbon – carbon single bonds – conformations of ethane and n-butane – conformational free energy – conformational isomers and atropisomers – population of conformers – influence of dipole – dipole repulsion, van der Waals attractive force, intramolecular H-bonding on the stability of conformers.

Conformational analysis of cyclohexane systems – stability and isomerism in mono and di substituted cyclohexane – flexible conformers – conformational analysis of cyclohexane and its derivatives, cyclohexanones – alkyl ketone effect -  $\alpha$  - halocyclohexanones – anomeric effect, Decalins.

**Unit II** Dynamic stereochemistry conformation and reactivity

Conformation and reactivity in acyclic systems – stereo electronic and steric factors – simple examples illustrating E2 and cis eliminations, intramolecular rearrangements and neighbouring group participation, Curtin-Hammett principle. Winstein Elliel Equation, Steric assisted and steric hindered reaction

Simple reactions illustrating stereo and stereoelectronic factors – esterification, oxidation, nucleophilic substitution at ring carbons and elimination reactions - reactions involving

intramolecular rearrangements – formation and cleavage of epoxides and neighbouring group participation – reactions of enols and enolates

### **Unit III** Reagents in organic synthesis

Use of the following reagents in organic synthesis and functional group transformation – Dicyclohexylcarbodiimide, 1,3 dithiane (reactive umpolung), trimethylsilyl iodide, tri-n-butyltin hydride, Woodward and Prevost hydroxylation, DDQ Wilkinson's Catalyst – Wittig reaction

### **Unit IV** Oxidation and Reduction

Oxidation of organic compounds with reagents based on peroxides, peracids, ozone, oxides of osmium, chromium, iodine and selenium dioxide

Reduction of organic compounds with reagents based on  $\text{LiAlH}_4$ ,  $\text{NaBH}_4$ , Raney Ni hydrazine, formic acid and dissolving metals. Clemmenson reaction, Wolf Kishner reduction, Birch Reduction.

### **Unit V** Asymmetric Synthesis

Importance of asymmetric synthesis – problems with resolution methods – optical purity - enantiomeric excess – diastereomeric excess – chiral, substrate controlled, auxiliary controlled, catalyst controlled and solvent controlled asymmetric synthesis, example for each case, synthesis of longifolene by EJ Corey method.

#### **Books for study**

- 1.E.L.Eliel, Stereochemistry of Carbon Compounds, McGraw Hill, 1962.
- 2.V.M.Potapov, Stereochemistry, MIR Publishers, Moscow 1979.
- 3.D.Nasipuri, Stereochemistry of Organic compounds, 2<sup>nd</sup> Edn, New Age International, New Delhi, 1972.

#### **Books for reference**

- 1 E.L.Eliel , N.C.Allinger, S.J.Angyal and G.A.Morrison, Conformational analysis, Interscience, New York, 1965.
- 2.C.Djerassi, Optical Rotatory Dispersion – Application to Organic Chemistry, McGraw Hall, 1960.
- 3 R.E.Ireland, Organic Synthesis, Prentice Hall, 1969.
4. S.Turner, Design of Organic Synthesis, Elsevier, 1976.

#### **Online Resource**

1. <http://www.fccj.us/chm2210/2210pptmenu.html>
2. <http://courses.washington.edu>
3. <https://chem.libretexts.org>

## INORGANIC CHEMISTRY – II

**Programme: M.Sc.,**

**Subject: Chemistry**

**Semester: I**

**Course: Inorganic Chemistry II**

**Course Type: Core Paper-I**

**Credits: 5**

**Hours Required: 5Hrs / Week**

**CIA:25 /CA75**

### Course Outcomes:

After completion of the course, certain outcomes are expected from the learners.

Description of COs	Bloom's Taxonomy Level
Understanding and explaining crystal field theory, crystal field splitting in complexes, its limitations,	Understanding (Level 2)
Deriving the Orgel and Tanabe, Sugano diagram, effect of Jahn – Teller distortion and spin-orbit coupling on absorption spectra	Creation (Level 6)
Analysing and categorizing the mechanical aspects of organometallic complexes	Analysis (Level 4)
Describing trans effect, theories of trans effect and redox reactions	Understanding (Level 2)
Applying the interpretation the electronic spectra of coordination complexes.	Application (Level 3)

## COURSE CONTENT

### Unit I Chemistry of Coordination Compounds

Brief review of the general characteristics of transition elements, nomenclature of coordination complexes, Isomerism in coordination compounds, types of ligands and chelate effect, stepwise and overall formation constants-determination of stability constant by Job's continuous variation method., VB theory and CFT - Splitting of d-orbitals under different geometries – CFSE – evidence for CFSE-factors affecting CFSE – spectrochemical series – Jahn-Teller distortion- application of d-orbital splittings to explain magnetic properties, spin, Limitations of CFT – MO theory – sigma – and pi-bonding in complexes – Nephelauxetic effect

### Unit II Electronic Spectra of Metal Complexes

Term symbols for atoms and ions – splitting of orbitals and terms in crystal fields – characteristics of d-d transitions – energy levels – Orgel and Tanabe – Sugano diagram – effect of Jahn – Teller distortion and spin-orbit coupling on absorption spectra – crystal field spectra of transition metal complexes – calculation of  $10Dq$  and  $\beta$  for Co(II) ( $O_h$  and  $T_d$ ) and Ni(II) ( $O_h$ ) complexes- charge transfer spectra of bipyridine and related diimine systems

ORD and CD: Chirality and the special nomenclature of chiral coordination compounds - optical activity, ORD and CD – Cotton effect – absolute configurations of chiral coordination compounds

### **Unit III Inorganic Reaction Mechanism**

Electron transfer reactions: Outer-sphere and inner sphere electron transfer reactions – The Marcus theory – non-complementary reactions – synthesis of coordination compounds by electron transfer reactions

Substitution reactions Trans Effect, substitution reactions of square planar complexes of Pt(II) and other  $d^8$  metal complexes – significance of trans-effect – substitution reactions of octahedral complexes – acid and base hydrolysis reactions – anation reactions, the template effect and macrocyclic ligands.

### **Unit IV Organometallics**

The 18 electron rule – applications and limitations – Isolobal concept and its usefulness Hapticity, Metal alkyl and aryls – olefin and acetylene complexes – Zeise salt – Dewar-Chatt approach to bonding in olefins & cyclobutadiene complexes, cyclopentadiene and benzene complexes of transition metals (preparation, bonding and reactions), – Fluxional molecules. Homogeneous catalysis involving organometallics – oxidative addition and reductive elimination reactions – hydrogenation, isomerization and hydroformylation of olefins – carbonylation of methanol, oxidation of olefins (Wacker process) - heterogeneous catalysis – Ziegler-Natta polymerization of propylene.

### **Unit V Pi-acceptor Complexes**

Synthesis, structure and bonding of mono nuclear and poly-nuclear carbonyls – nitrosyl complexes – dinitrogen complexes – metal carbonylato complexes, carbonyl hydrides and complex metal cyanides.

### **Books for study**

1. J.D. Lee, Concise Inorganic Chemistry, 5<sup>th</sup> Ed, Wiley, 1999.
2. J.E. Huheey, Inorganic Chemistry, 3<sup>rd</sup> Ed., Harper & Row publisher, 1983
3. D.F. Shriver, P.W. Atkins, Inorganic Chemistry, 3<sup>rd</sup> Ed, 1999

### **Books for reference**

1. D.E. Douglas, D.H. McDaniel, J.J. Alexander, Concepts and Models in Inorganic Chemistry, 3<sup>rd</sup> Ed. 1994.
2. F.A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry, 4<sup>th</sup> Ed., John Wiley & Sons, 1986
3. S.F.A. Kettle, Physical Inorganic Chemistry – A Coordination Chemistry Approach,

Oxford University Press, 1996.

4. A.G. Sharpe, Inorganic Chemistry, Pearson Education, 2008.

**Online resources:**

1. <https://nsufl.libguides.com/cnso-inorgchem/websites>

2. <https://www.tandfonline.com>

## PHYSICAL CHEMISTRY – II

Programme: M.Sc.,

Subject: Chemistry

Semester: I

Course: Inorganic Chemistry II

CourseType: Core Paper-I

Credits:5

Hours Required:5 Hrs / Week

CIA:25 /CA:75

### Course Outcomes:

After completion of the course, certain outcomes are expected from the learners.

Description of COs	Bloom's Taxonomy Level
Appreciating and analyzing the importance of the reactions in surface and catalysis.	Analysis (Level4)
Evaluating commutation relation between total orbital angular momentum operator and its components.	Evaluation (Level5)
Applying the uses of polymer chemistry in future studies	Application (Level 3)
Using mathematical techniques in linear algebra for eigen values and eigen vectors and first and second order differential equations in quantum chemistry and in physical and theoretical chemistry	Application (Level 3)
Solving all the model problems in quantum mechanics for which exact analytical methods	Creation (Level 6)

## COURSE CONTENT

### Unit I Quantum Theory – I

Planck's quantum theory – Bohr atom model - Wave – Particle duality – Uncertainty Principle – Operators and commutation relations – Sums and product of operator, commutator, linear and non-linear operator, Hermitian and Hamiltonian operator, Postulates of quantum mechanics and Schrodinger equation – eigen functions and eigen value, - Free particle – Particle in a box – degeneracy-one and three. dimensional, distortion of the box and Jahn-Teller effect, quantum numbers, zero-point energy, - orthogonalisation and normality finite potential barrier – tunneling

### Unit II Quantum Theory – II

Derivation of angular momentum operator, Rigid rotator-Harmonic oscillator. The hydrogen atom – space quantization of electronic orbits – angular and radial part, electron spin - Approximate methods of solving the Schrodinger equation – The perturbation and variation methods – Application to He atom - Angular momentum– spin orbit interaction – vector model of the atom – term symbols - Pauli exclusion principle Slater determinant. Atomic Structure Calculation

### Unit III Quantum Theory – III

Molecular Orbital and valence bond theory of molecules: The Born–Oppenheimer approximation, MO treatment of  $H_2^+$ , and MO and VB treatment of  $H_2$  molecule – comparison of MO and VB methods. Bonding in homo and hetero nuclear diatomics (HF, CO, NO) – polyatomic molecules concept of hybridization -Huckel theory of conjugated systems - application to ethylene, butadiene.

#### **Unit IV Surface Chemistry and Catalysis**

Surface Phenomena: Physisorption and chemisorptions ,solid- liquid interfaces – contact angle and wetting, Adsorption from solution, , Gibbs adsorption isotherm — solid-gas interface — Freundlich, Langmuir, Temkin, BET isotherms – surface area determination.

Homogeneous catalysis – Acid-base catalysis – Acidity function – Enzyme catalysis – Michaelis–Menten kinetics. Kinetics of bimolecular surface reactions involving adsorbed species – Langmuir-Hinshelwood mechanism, Langmuir – Rideal mechanism – Rideal –Eley mechanism. Basic aspects of semiconductor catalysis and applications

Solar energy conversion – Photogalvanic cell – Photoelectrochemical cells – Electrolysis of water.

#### **Unit V Polymer Chemistry**

Overview of polymers – Structure and classification of polymers – Degree of polymerization, Kinetics and mechanism of free radical and ionic polymerizations - Coordination polymerization, Zeigler–Natta catalysis Condensation – Self catalysed and Non-catalysed polycondensation, Copolymerization – Co-polymer - Equation and significance, Molecular weight of polymers– Determination of molecular weight – Light scattering and viscosity methods - Gel permeation chromatography.

Stereoregularity of polymers- significance of  $T_g$  and  $T_m$

#### **Books for study**

1. A.K. Chandra, Introductory Quantum Chemistry, 4<sup>th</sup> Ed., Tata McGraw Hill, 2009.
2. I.N. Levine, Quantum Chemistry, Allyn and Bacon, 1983
3. P.W. Atkins, Molecular Quantum Mechanics, 2<sup>nd</sup> Edn, Oxford Univ. Press, 1987
4. F.W. Billmeyer, Jr., A Text Book of Polymer Science, John Wiley, 1971.
5. V.R. Gowariker, N.V. Viswanathan, J. Sreedhar, Polymer Science, New Age Publishers, 1986.
6. P.W. Atkins, Physical Chemistry, 7<sup>th</sup> Ed., Oxford University press, 2002.
7. S. Glasstone, Text book of Physical Chemistry, McMillan, 1974.

#### **Books for Reference**

1. D.A. McQuarrie, D. Simon, Physical chemistry, A Molecular Approach, Viva Books

Pvt. Ltd, 2003.

2. D.A. Mcquarrie, Quantum Chemistry, University Science Books, 1998.
3. F.L. Pillar Elementary Quantum Chemistry, McGraw Hill, 1968.
4. J.P. Lowe and K.A.Peterson, Quantum Chemistry, 3<sup>rd</sup> Edn., Elsevier 2006

**Online resource**

1.<https://chem.libretexts.org>

2. [https://en.wikipedia.org/wiki/Quantum\\_chemistry](https://en.wikipedia.org/wiki/Quantum_chemistry)

## INORGANIC CHEMISTRY PRACTICALS

**Programme: M.Sc.,**

**Subject: Chemistry**

**Semester: II**

**Course: Inorganic chemistry Practical**

**Course Type: Core Paper-I**

**Credits: 5**

**Hours Required: 5Hrs/week**

**CIA:25 / CA:75**

### **Course Outcomes:**

After completion of the course, certain outcomes are expected from the learners.

<b>Description of COs</b>	<b>Bloom's Taxonomy Level</b>
Estimating the metals and alloys by using quantitative methods	Analysis (Level 4)
Analyzing the ores and pharmaceutical preparations quantitatively.	Analysis (Level 4)
Presenting scientific and technical information resulting from laboratory experimentation in both written and oral formats.	<b>Creation (Level 6)</b>
Working effectively and safely in laboratory environment	<b>Creation (Level 6)</b>
Applying the skills in future studies	Application (Level 3)

## COURSE CONTENT

### **Practical – A : Qualitative Analysis**

Less common metal ions – Mo, Se, Te, Ce, W, Ti, Zr, Th, U, V, Li (two metal ions in cationic and anionic forms)

### **Practical – B : Quantitative Analysis**

- a) EDTA titrations : Zn(II), Mg(II), Cu(II) and Ni(II)  
Redox titrations : Fe(II) vs. Ce(IV) , Fe(II) vs. dichromate  
NO<sub>2</sub><sup>-</sup> vs. Ce(IV)
- c) Spectrophotometric methods of analysis : Fe(II) , Cu(II) .

### **Books for study**

1. Vogel's Qualitative Inorganic Analysis

### **Books for reference**

1. Practical Inorganic Chemistry by Gulati and Shikha and Sharma and JL and Manocha and Shagun

## ANALYTICAL TECHNIQUES

**Programme: M.Sc.,**

**Subject: Chemistry**

**Semester: I**

**Course: Analytical technique**

**Course Type: Core Paper-I**

**Credits:5**

**Hours Required: 5Hrs / week**

**CIA:25 /CA:75**

### **Course Outcomes:**

After completion of the course, certain outcomes are expected from the learners.

<b>Description of COs</b>	<b>Bloom's Taxonomy Level</b>
Solving problems based on various analytical concepts	Creation (Level 6)
Designing experiments with improved sample preparation, new measurement procedures and tools	Creation (Level 6)
Quantifying analytes with proper data handling and analysis	Analysis (Level 4)
Evaluating thermo analytical technique	Evaluation (Level 5)
Using the electro-analytical studies for research	Application (Level 3)

## COURSE CONTENT

### **UNIT I Chromatography – I**

**HPLC:** Introduction – Column Packing Materials – Solvent – Detectors – Recorder – Terms and Definitions used in HPLC analysis and applications.

**Gas Chromatography:** Introduction – Retention Time – Retention Volume – Efficiency – Carrier Gases – Preparation of Columns – Solid Supports – Stationary Phases Detectors – Temperature Effect – Quantitative and Qualitative analysis and applications.

### **UNIT – II**

#### **Chromatography – II Gel Permeation Chromatography: (GPC)**

Introduction – Types of gels – Selection of gels – Gel Preparation – Drying of gels – Packing of the Column Application of the sample – Resolution – Detectors and Applications.

#### **Gas Chromatography Mass Spectrometry: (GCMS)**

Introduction – Separators – Carrier gas – Sample Injection – Analyzer and Applications.

#### **Liquid Chromatography Mass Spectrometry: (LCMS)**

Introduction – Ionization – Belt Interface – Instrumentation and Applications.

### **Unit III**

#### **Electroanalytical methods**

**Amperometry**-Principles and applications, amperometric titration with examples- comparison with other titration methods-Basic principles of electrogravimetry

**Coulometry:** principles- coulometry at controlled potential- coulometry at constant current- coulometric titrations-advantages and applications

**Cyclic Voltammetry:** Principles and simple analytical applications – Interpretation of cyclic voltammogram.

#### **Unit IV**

##### **Spectrometry and thermal methods**

Atomic absorption spectrophotometer(AAS)- principle, instrumentations and applications- types of interferences. Flame Emission spectroscopy (FES)- theory, instrumentation and applications, Difference between AAS and FES. Thermal methods of Analysis- principle, instrumentations and applications of TG, DTA and DSC-thermograms of calcium oxalate and  $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$

#### **Unit V**

##### **Surface analysis and XRD**

Photoelectron spectroscopy-theory-photo sources-electron analyzers - resolution-assignment of bands-Koopman's theorem-principle, instrumentation and applications of UV, XPS and ESCA, Auger effect

##### **Books for study**

1. D. A. Skoog, F. J. Holler and S. R. Crouch, Principles of Instrumental Analysis, 6th Edition, Brooks/Cole Cengage Learning, Belmont, CA, 2007
2. H. H. Willard, L. L. Merrin, Jr., J. A. Dean, and F. A. Senle, Jr., Instrumental Methods of Analysis: Wadsworth, 7th Edition, Belmont., 1989

##### **Books for reference**

1. D. C. Harris, Quantitative Chemical Analysis, 4th Ed., W. H. Freeman, 1995
2. G. D. Christian & J. E. O'Reily, Instrumental Analysis, 2nd Ed., Allyn & Balon, 1986.
3. P.J. Wheatley, The Determination of Molecular Structure, (Unit V), Oxford University Press, 1968.
4. 4.M.P. Seah, D. Briggs, Practical Surface Analysis by Auger and X-ray Photoelectron Spectroscopy, 2<sup>nd</sup> Ed., Wiley, 1992

##### **Online resource**

1. <http://web.uni-plovdiv.bg>
2. <https://onlinelibrary.wiley.com>

**SEMESTER – III**  
**ORGANIC CHEMISTRY – III**

**Programme: M.Sc.,**

**Subject: Chemistry**

**Semester: III**

**Course: Organic Chemistry II**

**Course Type: Core Paper-I**

**Credits:5**

**Hours Required: 5Hrs / week**

**CIA: 25 / CA:75**

**Course Outcomes:**

After completion of the course, certain outcomes are expected from the learners.

<b>Description of COs</b>	<b>Bloom's Taxonomy Level</b>
Applying the effect of structure on chemical shift and coupling constants.	Application (Level 3)
Constructing splitting diagrams and be able to measure coupling constants, and NMR spectrum, or predict coupling constants	Creation (Level 6)
Describing and explaining photochemical and photophysical processes using Norrish, Buterno Puchi diagram and their quantum yield expressions	Comprehension (Level 2)
Recognizing and know how to test for exchangeable hydrogens in a molecule.	Knowledge (Level 1)
Deducing unknown structures and fully assign an IR spectrum to the structure.	Analysis (Level 4)

**COURSE CONTENT**

**Unit I**

**Organic Photochemistry**

Thermal versus photochemical reactions, basic concepts of organic photochemistry, Jablonski diagram – energy transfer mechanism – photochemical reactions of saturated ketones – Norrish type I and II reactions – photoreduction – Paterno - Buchi reaction – reaction of  $\alpha$ ,  $\beta$  unsaturated ketones – isomerisations – photochemistry of simple olefins – cis-trans isomerisation – di- $\pi$  methane rearrangement – photochemical oxidations – oxidative coupling – photochemistry of arenes.

**Unit II**

**Pericyclic reactions**

Definition of pericyclic reactions – electrocyclic, cycloaddition and sigmatropic reactions – selection rules and stereochemistry for thermal and photochemical reactions – explanation on the basis of (i) FMO approach (Fukui), (ii) orbital correlation diagram approach (Woodward and Hoffmann) and (iii) aromatic transition state approach (Dewar and Zimmerman) Taking simple systems as example. Diels-Alder reaction, ene reaction, Sommelet – Hauser, Cope and

Claisen rearrangements.

### **Unit III**

#### **Application of UV, IR and Mass Spectrometry in organic chemistry**

UV spectra – types of excitation or transition probability – chromophores and auxochromes – factors affecting intensity and position of absorption bands – Dienes, Polyenes and Enones – Woodward Fischer rules.

IR Spectra – Hooke's law – factors affecting vibrational frequencies – characteristic group frequencies – Finger print region.

Mass spectrometry – basic principles – molecular ion peak, parent peak, fragments, metastable peak, isotope peaks – determination of molecular weight and molecular fragment – fragment pattern of simple organic molecules – Mc lafforty rearrangement – Retero Diels Alder reaction.

### **Unit IV**

#### **Applications of NMR spectroscopy in organic structural determination**

$^1\text{H}$  NMR spectroscopy – origin of NMR spectra – chemical shift – number of signals – peak areas – multiplicity – geminal, vicinal and long range couplings – factors affecting chemical shifts and coupling constants, Karplus equation, AX, AX<sub>3</sub>, AB<sub>2</sub>, ACMX PATTERNS first order spectra, Simplification of complex spectra.

$^{13}\text{C}$  NMR spectroscopy: Broadband and Off resonance decoupling, comparison of  $^1\text{H}$  and  $^{13}\text{C}$  NMR – factors affecting intensity of signals – chemical shifts -  $\gamma$  - gauche effect  
2D Techniques:  $^1\text{H}$ - $^1\text{H}$  COSY ,  $^1\text{H}$ - $^{13}\text{C}$  COSY .

### **Unit V**

#### **Organic Synthesis**

Importance of synthesis – carbon-carbon bond making reactions – functional group modifications – retrosynthetic analysis – synthons and synthetic equivalents – nucleophilic, electrophilic, electroneutral and free radical synthons – retron, partial retron and super retron - Chiron – umpolung – protection and deprotection – product, chemo, regio and stereoselectivities.

One and two group disconnections – Diels Alder reactions – Robinson annulation method – 1,2- 1,3- 1,4- 1,5- and 1,6- difunctional compounds

#### **Books for study**

- 1.Y.R.Sharma Elementary Organic Spectroscopy
- 2.P.S.Kalsi Organic spectroscopy
- 3.V.K.Aluwaliya Organic synthesis

### **Books for Reference**

1. P.M. Silverstein, F.X. Wester, Spectroscopic Identification of Organic Compounds, 6<sup>th</sup> Ed., Wiley 1998.
2. J. Mohan, Organic Spectroscopy Principles and Applications, 2<sup>nd</sup> Ed., CRC, 2004.
3. W. Kemp, Organic Spectroscopy, 3<sup>rd</sup> Ed., MacMillon, 1994.
4. D.L. Pavia, G.M. Lampman, G.S. Kriz, Introduction to Spectroscopy, 3<sup>rd</sup> Ed., Brooks Cole, 2000.

### **Online resource**

1. [https://en.wikibooks.org/wiki/Organic\\_Chemistry/Spectroscopy](https://en.wikibooks.org/wiki/Organic_Chemistry/Spectroscopy)
2. <https://chem.libretexts.org>

## INORGANIC CHEMISTRY – III

**Programme:** M.Sc.,

**Subject:** Chemistry

**Semester:** I

**Course:** Inorganic Chemistry II

**Course Type:** Core Paper-I

**Credits:** 5

**Hours Required:** 5Hrs/week

**CIA:25 / CA:75**

### Course Outcomes:

After completion of the course, certain outcomes are expected from the learners.

Description of COs	Bloom's Taxonomy Level
Applying NMR, IR, MS, UV-Vis spectroscopic techniques in solving structure of organic molecules and in determination of their stereochemistry.	Application (Level 3)
Evaluating the concept of inorganic photochemistry	Evaluation (Level 5)
Using these spectroscopic techniques in their research	Application (Level 3)
Elucidating the structure of simple molecule by using Infrared spectra	Creation (Level 6)
Describing the spectral concepts of $^1\text{H}$ , $^{19}\text{F}$ , $^{31}\text{P}$ , $^{13}\text{C}$ interpretation and applications and their bonding patterns	Comprehension (Level 2)

## COURSE CONTENT

### Unit I Infrared Spectroscopy

Spectroscopy in the structural elucidation of simple molecules like  $\text{N}_2\text{O}$ ,  $\text{ClF}_3$ ,  $\text{NO}_3^-$ ,  $\text{ClO}_4^-$  – effect of coordination on ligand vibrations – uses of group vibrations in the structural elucidation of metal complexes of urea, thiourea, cyanide, thiocyanate, nitrate, sulphate and dimethyl sulfoxide

### Unit II NMR Spectroscopy

Examples for different spin systems – chemical shifts and coupling constants (spin-spin coupling) involving different nuclei ( $^1\text{H}$ ,  $^{19}\text{F}$ ,  $^{31}\text{P}$ ,  $^{13}\text{C}$ ) interpretation and applications to inorganic compounds- NMR spectra of  $\text{P}_4\text{S}_3$ ,  $\text{H}_3\text{PO}_3$ ,  $\text{H}_3\text{PO}_2$  and  $\text{HPF}_2$ .  $^{19}\text{F}$  NMR spectra of  $\text{ClF}_3$ ,  $\text{BrF}_3$  and equimolar mixture of  $\text{TiF}_6$  and  $\text{TiF}_4$  in ethanol – Effect of quadrupolar nuclei on the  $^1\text{H}$  NMR spectra, Satellite spectra.

Systems with chemical exchange - study of fluxional behavior of molecules NMR of paramagnetic molecules – isotropic shifts contact and pseudo-contact interactions – Lanthanide shift reagents.

### Unit III EPR Spectroscopy

Theory of EPR spectroscopy - Spin densities and McConnell relationship –presentation of the spectrum-hyperfine splitting, Applications of ESR to some simple systems such as  $\text{CH}_3$ , *p*-benzosemiquinone,  $\text{Xe}_2^+$  - Factors affecting the magnitude of *g* and *A* tensors in metal species -

Zero-field splitting and Kramers degeneracy – Spectra of VO(II), Mn(II), Fe(III), Co(II), Ni(II) and Cu(II) complexes

### **Mossbauer Spectroscopy**

Theory-Doppler effect - isomer shift-quadruple splitting-magnetic hyperfine splitting-application of MB spectroscopy to inorganic compounds

### **Unit IV Nuclear Chemistry**

Properties of nucleus – different types of nuclear forces – liquid drop model, shell model of nucleus – nuclear reactions induced by charged particles – Q value – nuclear reaction cross section, significance and determination – theory of nuclear fission – reactor and its components – production of feed materials for nuclear reactors – disposal of radioactive wastes – nuclear fusion, stellar energy. Application of radioisotopes in agriculture, industry and medicine – neutron activation analysis – hot atom chemistry.

### **Unit V Inorganic Photochemistry**

Elementary ideas on the photosystems I and II - Photochemistry of Cr(III), Co(III) and Ru(II) - coordination compounds – photoaquation – photoanation – photoisomerisation – photo redox reactions – charge transfer photo chemistry – photosensitization – solar energy conversion – photogalvanic cell – splitting of water to evolve hydrogen and oxygen – photochemistry of Pt(II) and Pt(IV) complexes

### **Books for study**

1. R.S. Drago, Physical Methods in Inorganic Chemistry, 3<sup>rd</sup> Ed., Wiley Eastern Company
2. K.K. Rohatgi-Mukherjee, Fundamentals of Photochemistry, Tata-McGraw Hill, 1981.
3. E.A.V. Ebsworth, Structural Methods in Inorganic Chemistry, 3<sup>rd</sup> Ed., ELBS, 1987.
4. Arniger, Nuclear Chemistry

### **Books for Reference**

1. R.S. Drago, Physical Methods in Chemistry, W. B. Saunders Company, 1992.
2. J. Lewis, R.G. Wilkins, Modern Coordination Chemistry, Inter Science publisher, 1960.
2. K.K. Rohatgi-Mukherjee, Fundamentals of Photochemistry, Tata-McGraw Hill, 1981.

### **Online Resource**

- 1.[https://wiki.ubc.ca/The\\_Role\\_of\\_Spectroscopy\\_in\\_Inorganic\\_Chemistry](https://wiki.ubc.ca/The_Role_of_Spectroscopy_in_Inorganic_Chemistry)
- 2.<https://www.chem.ualberta.ca/~inorglab/spectutor.htm>

## PHYSICAL CHEMISTRY – III

**Programme:** M.Sc.,

**Subject:** Chemistry

**Semester:** I

**Course:** Physical Chemistry III

**Course Type:** Core Paper-I

**Credits:**5

**Hours Required:** 5Hrs / week

**CIA: 25 / CA: 75**

### Course Outcomes:

After completion of the course, certain outcomes are expected from the learners.

Description of COs	Bloom's Taxonomy Level
Evaluating the concept of vibrating, rotating spectra.	Evaluation (Level 5)
Describing the basic theory of Nuclear Magnetic Resonance (NMR) Spectroscopy	Comprehension (Level 2)
Applying the basic principles and application of Electron spin resonance (ESR) spectroscopy for the structural elucidation of compounds.	Application (Level 3)
Determining the vibrations for a triatomic molecule and identify whether they are infrared-active.	Analysis (Level 4)
Calculating the symmetry elements and symmetry operations, point groups and character table	Creation (Level 6)

## COURSE CONTENT

### Unit I Group Theory : Concepts

Elements of symmetry – point group classification of molecules – definition and theorems of group – properties of group with examples - symmetry operations as elements of group – group multiplication table – similarity transformations – sub groups – classes – representation of groups - reducible and irreducible representations – Great orthogonality theorem (derivation and proof excluded) – character table for H<sub>2</sub>O and NH<sub>3</sub> molecules – format and significance – direct products and simplified procedure for generating and factoring total representations. Symmetry adapted linear combinations – projection operators.

### Unit II Group theory : Applications

Molecular vibrations and their symmetry types in typical molecules – IR and Raman activity – bonding with central atom and formation of hybrid atomic orbitals in molecules such as BF<sub>3</sub>, (PtCl<sub>4</sub>)<sub>2</sub>CH<sub>4</sub> – simplification of MO calculations – naphthalene, benzene – symmetries of molecular orbitals and electronic configurations – group theoretical selection rules – vanishing matrix elements selection rules for electronic transitions – electronic spectra of the carbonyl chromophore.

### Unit III Spectroscopy – I

General features of spectrum – Experimental techniques – Intensities of spectral lines and

linewidths - Rotational spectra - Vibrational spectra – Rotation–Vibration spectra of diatomic and polyatomic molecules – Fermi resonance – Basic concepts of FTIR – Raman spectroscopy – Rotational Raman and vibrational Raman – Resonance Raman and Laser Raman – Electronic spectra of diatomic molecules – Franck-Condon principle – Vibrational and rotational fine structure – Fortrat diagram – Predissociation.

#### **Unit-IV Spectroscopy – II**

NMR – nuclear spins in a magnetic field – Zeeman effect – Larmor precession – Resonance phenomenon – Bloch equations – Spin - lattice and spin-spin relaxation times – Nuclear shielding and chemical shift – Spin-spin coupling – Basic principles of FT NMR – Inversion recovery and CPMG sequenced for  $T_1$  and  $T_2$  measurements – NMR instrumentation.

ESR – Electronic Zeeman effect – ESR spectrum of hydrogen atom (first order treatment) - g factors – Hyperfine constants – ESR of organic radicals in solution – McConnell's relation – ESR instrumentation.

#### **Unit V Statistical Thermodynamics**

Thermodynamics probability and entropy – Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac statistics and applications, - partition function and entropies for translational, rotational, vibrational and electronic motions of monoatomic and diatomic molecules – calculations of thermodynamic functions and equilibrium constants – specific heat of solids – Einstein and Debye theories.

#### **Books for study**

1. F.A. Cotton, Chemical Applications of group Theory, 3<sup>rd</sup> Ed., Wiley Eastern, 2004.
2. R.L. Carter, Molecular Symmetry and Group Theory John Wiley, 1998.
3. C.N. Banwell, E. McCash, Fundamentals of molecular Spectroscopy, 4<sup>th</sup> Ed., TMH, 2008.
4. B.P. Straughan, S.Walker Spectroscopy Vol.3, Chapman Hall, 1976.
5. G.M. Barrow, Introduction to Molecular Spectroscopy, McGraw Hill, 1964.
6. P.K. Ghosh, Introduction to Photoelectron Spectroscopy, John Wiley, 1989.
7. P.W. Atkins, Physical Chemistry, 7<sup>th</sup> Ed., Oxford University press, 2002.

#### **Books for Reference**

1. R.L. Flurry, Jr, Symmetry Groups – Prentice Hall, New Jersey 1980.
2. B.E. Douglas and C.A. Hollingsworth, Symmetry in Bonding and Spectra – An Introduction, Academic Press, 1985.
3. S.F.A. Kettle, Symmetry and Structure, John Wiley & Sons, 1985

#### **Online resource**

1. <https://www.chem.fsu.edu>
2. <http://contents.kocw.or.kr>
3. <https://chem.libretexts.org>

## PHYSICAL CHEMISTRY PRACTICALS

**Programme: M.Sc.,**

**Subject: Chemistry**

**Semester: III**

**Course: Physical chemistry Practicals**

**CourseType: Core Paper-I**

**Credits: 5**

**Hours Required: 5Hrs / week**

**CIA:25 / CA:75**

### **Course Outcomes:**

After completion of the course, certain outcomes are expected from the learners.

<b>Description of COs</b>	<b>Bloom's Taxonomy Level</b>
Setting up of different electrochemical cells	Creation (Level 6)
Analyzing the dissociation constant and solubility product by conductometry and potentiometry respectively	Analysis (Level 4)
Identifying the thermodynamics of simple systems	Analysis (Level 4)
Assessing and adopting the conductometric methods to verify the theories	Application (Level 3)
Demonstrating the practical to others	Creation (Level 6)

### **COURSE CONTENT**

Any twenty experiments out of the following experiments (to be decided by the course teacher):

1. Kinetics – Acid Hydrolysis of Ester – Comparison of strength of acids.
2. Kinetics – Acid Hydrolysis of Ester – Determination of Energy of Activation ( $E_a$ ).
3. Kinetics – Saponification of Ester – Determination of  $E_a$  by conductometry.
4. Kinetics – Persulphate – Iodide Reaction – Determination of order, effect of Ionic strength on rate constant.
5. Polymerization – Rate of polymerization of acrylamide.
6. Distribution Law – Study of iodine – Iodide equilibrium.
7. Distribution Law – Study of Association of Benzoic Acid in Benzene.
8. Study of phase diagram of two components forming simple eutectic.
9. Study of phase diagram of two components forming a compound.
10. Determination of molecular weight of substances by TT measurements.
11. Determination of Critical Solution Temperature of phenol water system and effect of impurity on SCT.
12. Adsorption – oxalic Acid\Acetic Acid on charcoal using Freundlich isotherm.
13. Conductometry – Acid – alkali titrations.
14. Conductometry – precipitation titrations.
15. Conductometry - Displacement titrations.

16. Conductometry – Determination of dissociation constant of weak acids.
17. Conductometry – Solubility product of sparingly soluble silver salts.
18. Verification of Onsager equation – conductivity method.
19. Determination of degree of hydrolysis and hydrolysis constant of a substance.
20. Potentiometric titrations – Acid alkali titrations.
21. Potentiometric titrations – Precipitation titration.
22. Potentiometric titrations – Redox Titrations.
23. Potentiometry – Determination of dissociation constant of weak acids.
24. Potentiometry- Determination of solubility product and pKa

### **Books for study**

1. B. Viswanathan and P. S. Raghavan, Practical Physical Chemistry, Viva Books, 2009
2. Practical Physical Chemistry 1st Edition 2017 by Gupta, Renu, New Age International (P) Ltd Publishers

### **Reference Books**

1. B.P. Levitt, Ed., Findlay's practical Physical Chemistry, 9<sup>th</sup> Ed., Longman, 1985.
2. J.N. Gurtu, R. Kapoor, Advanced Experimental Chemistry, Vol.I, S.Chand & Co., 1987.

### **Online Resources**

1. <https://people.ok.ubc.ca/pphillips/DRAFT%20464%20Manual.pdf>
2. <https://pubs.acs.org/doi/abs/10.1021/ed013p250.2>

## ENVIRONMENTAL CHEMISTRY AND GREEN CHEMISTRY

**Programme:** M.Sc.,

**Subject:** Chemistry

**Semester:** III

**Course:** Environmental Chemistry and Green Chemistry

**Course Type:** Core Paper-I

**Credits:** 5

**Hours Required:** 5 Hrs / week

**CIA:** 5 **CA:** 5

### Course Outcomes:

After completion of the course, certain outcomes are expected from the learners.

Description of COs	Bloom's Taxonomy Level
Analysing the effect of Pollution and its prevention measures	Analysis (Level 4)
Designing the bio-catalytic reactions	Creation (Level 6)
Exploring the causes of global warming and its effects	Analysis (Level 4)
Applying the control and remedial measures of green house effect	Application (Level 3)
Evaluating about the various analytical green methods and protecting the environment	Evaluation (Level 5)

## COURSE CONTENT

### Unit I – Water Pollution

Types of water pollution, -Physical, chemical and biological types, ground water and surface water pollution – sources and harmful effects – sources and effects of major water pollutants – inorganic pollutants – oxygen demanding wastes - organic pollutants – plant nutrients – detergents – radioactive wastes – nuclear pollution – sources effects of ionizing and non-ionizing radiation. Significance of various water pollutants- thermal pollution

### Unit II – Air Pollution

Atmosphere-structure – functions and photochemical reactions – sources of air pollution- natural and man made – acid rain, classification and effects of air pollutants – CO, CO<sub>2</sub>, SO<sub>2</sub>, SO<sub>3</sub>, NO and NO<sub>2</sub> – hydrocarbon as pollutant – reactions of hydrocarbons and effects – particulate pollutants – sources and effects of Organic particulate and Inorganic particulate Green House effect – impact on global climate – role of CFC's – ozone holes – effects of ozone depletion – smog-components of photochemical smog-effects of photochemical smog.

### Unit III – Pesticides and Soil Pollution

Soil Pollution: Sources, Types, Pesticides – classification, mode of action – toxic effects of chlorinated hydro carbons, organophosphorous compounds and carbamates – alternatives to chemical pesticides – (pheromones, Juvenile hormones, chemosterilization)

### Unit IV – Treatment of drinking water

Removal of suspended impurities, removal of micro-organisms, Treatment of Effluents, 1°

treatment,- Filtration, Coagulation, - 2<sup>o</sup> treatment –oxidation ponds- 3<sup>o</sup> treatment-reverse osmosis, electrodialysis- Nanofiltration. uses of

Treatment of water for Industrial purpose- Hardness-softening methods-Zeolite-Limo-soda-Ion Exchange methods.

### **Unit V Green Chemistry**

Green Chemistry - Definition, principles and requirements, water mediated reactions - solventless reactions – microwave assisted reactions – solid supported reactions – uses of ionic liquids and supercritical carbon dioxide reaction in organized media – calixarene, zeolites, cyclodextrin and other supramolecules as media for selection reactions - clay catalysed reactions – definitions and examples of multicomponents reaction and tandem reactions – atom economy reactions.

#### **Books for study**

1. Asim K.Das, Environmental Chemistry with Green Chemistry, Books & Allied (P) Ltd, Kolkata, 2012.
2. B.K.Sharma, Environmental Chemistry, Goel Publishers, 2001.

#### **Books for Reference**

1. A.K. De, Environmental Chemistry, New Age International, Fifth Edition, 2005.
2. C. J. Gonzalez, D. J. C. Constable, Green Chemistry and Engineering, A practical Design approach, Wiley Interscience, 2011
3. S. Parsons, B. Jefferson, Introduction to potable water treatment processes, Wiley – Blackwell, 2006.

#### **Online Resource**

1. <https://static1.squarespace.com>
2. [http://www.jlakes.org/config/hpkx/news\\_category/2015-06-03/ContaminatedSediments-2009.pdf](http://www.jlakes.org/config/hpkx/news_category/2015-06-03/ContaminatedSediments-2009.pdf)

**SEMESTER – IV**  
**CHEMISTRY OF NATURAL PRODUCTS AND**  
**BIO-INORGANIC CHEMISTRY**

**Programme:** M.Sc.,

**Subject:** Chemistry

**Semester:** IV

**Course:** Chemistry of Natural Products  
and Bioinorganic Chemistry

**Course Type:** Core Paper-I

**Credits:** 5

**Hours Required:** 5 Hrs / week

**CIA: 25 / CA: 75**

**Course Outcomes:**

After completion of the course, certain outcomes are expected from the learners.

<b>Description of COs</b>	<b>Bloom's Taxonomy Level</b>
Analyzing the essential Chemicals present in the natural products.	Analysis (Level 4)
Identifying, comparing and explaining aspects related to drug design, drug action	Analysis (Level 4)
Assigning the future research in DNA, RNA properties	Application (Level 3)
Evaluating the role of metal ions in biological system	Evaluation (Level 5)
Drawing and residing the structure of DNA, RNA, Steroids, fatty acids, alkaloids, terpenoids	Creation (Level 6)

**COURSE CONTENT**

**Unit I Proteins, peptides, Nucleic acid, Fats and Lipids**

Structure and properties of amino acids and proteins, Zwitterions and purification of proteins

Nucleic acids – nucleotides and nucleosides – structure of purine and pyrimidine bases;

Phosphodiester bond, double helical structure of DNA. Structure of RNA (tRNA)

Fatty acids - structure and classification, lipids classification and function (Simple, compound and derived lipids)

**Unit II Terpenoids**

Classification of terpenoids with examples – isoprene rules – General methods of structural determination of terpenes – structure and synthesis of *alpha*-pinene, cadinene, zingiberene and abietic acid

**Unit III Alkaloids**

General methods of structure analysis of alkaloids – Hoffmann, Emde and von Braun degradations – Structure and synthesis of quinine, papavarine, atropine, narcotine, reserpine and lysergic acid.

**Unit IV Steroids**

Types of steroids – structure, stereochemistry and synthesis of cholesterol – Structural features of bile acids – Sex hormones – androsterone, testosterone, estrone, estriol, estradiol, progesterone - Structure of ergosterol.

Circular birefringence, optical rotary dispersion, circular dichroism – Cotton effect curves – octant rule – axial haloketone rule - Applications of chiroptical properties in configurational assignments.

### **Unit V Bioinorganic Chemistry**

Metal ions in biological systems: heme proteins, hemoglobin, myoglobin, hemerythrin, hemocyanin, ferritin, transferrin, cytochromes and vitamin B12; Iron-sulphur proteins: rubredoxin, ferredoxin and model systems. Classification of copper proteins and examples - Electron transfer (Cu, Zn) – Blue copper proteins

Metalloenzymes: active sites, carboxy peptidase, carbonic anhydrase, superoxide dismutase, xanthine oxidase, peroxidase and catalase; photosynthesis, water oxidation, nitrogen fixation, nitrogenase; ion pump, metallodrugs.

#### **Books for study**

1. I.L. Finar, Organic Chemistry, Vol.II, ELBS 1985
2. S.J. Lippard, J.M. Berg, Principles of Bioinorganic Chemistry, Panima Publishing Company, 1977.
3. Gurdeep R Chatwal, Organic Chemistry Of Natural Products, Volume I , Himalaya Publishing House, 2009
4. L. Stryer, Biochemistry, 4<sup>th</sup> Ed., W. L. Freeman and Co, New York, 1995.
5. D. L. Nelson, M. M. Cox, Lehninger Principles of Biochemistry, 5<sup>th</sup> Ed.

#### **Books for reference**

1. W. Kaim, B. Schwederski, Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, John Wiley & Sons, 1994.
2. Bioinorganic Chemistry, Chem. Education, 62, No. 11, 1985.
3. G.L. Eichorn, Inorganic Biochemistry, Volumes 1 & 2, 2<sup>nd</sup> Ed., Elsevier, 1973.
4. J.N. Davidson, The Biochemistry of Nucleic acids, ELBS, 1965.

#### **Online resource**

1. <https://www.routledge.com/Introduction-to-Natural-Products-Chemistry/Xu-Ye-Zhao/p/book/9781439860762>
2. <https://lecturenotes.in/m/25725-chemistry-of-natural-products>

## NANOCHEMISTRY AND SUPRAMOLECULAR CHEMISTRY

**Programme:** M.Sc.,

**Subject:** Chemistry

**Semester:** I

**Course:** Nanochemistry and Supramolecular Chemistry

**Course Type:** Core Paper-I

**Credits:** 5

**Hours Required:** 5 Hrs / week

**CIA: 25 / CA:75**

### Course Outcomes:

After completion of the course, certain outcomes are expected from the learners.

Description of COs	Bloom's Taxonomy Level
Analyzing the core concepts in supramolecular chemistry and explain non covalent interactions, molecular recognition and self-assembly.	Analysis (Level 4)
Describing some of the applications of supramolecular chemistry including industrial applications and supramolecular catalysis	Comprehension (Level 2)
Applying the significance of nanoscale & its dimensions	Application (Level 3)
Evaluating knowledge of various characterization techniques	Evaluation (Level 5)
Applying the short term and longer term applications of nanomaterials	Application (Level 3)

## COURSE CONTENT

### Unit I Nanoscience and Nanotechnology

Definition of nanodimensional materials, Classification of Nanomaterials – Significance of surface to volume ratio, Size effects - Importance of Nanomaterials - - Simple examples of unique properties of nanosized materials - Elementary aspects of bionanotechnology - Some important recent discoveries in nanoscience and technology, Applications of Nanomaterials

### Unit II Carbon-based Nanomaterials

Carbon: Bonding in Carbon compounds, Discovery of Cubane, Fullerenes: synthesis, chemical reactions and properties, Carbon Nanotubes: Structure of Single-Walled Carbon nanotubes, physical properties of Single-Walled Carbon nanotubes, synthesis of Carbon nanotubes, growth mechanisms, chemical modification of Carbon nanotubes –Diamondoid Nanomaterials: diamondoids, thin diamond films (and other ultrahard substances) – Chemical modification of CVD Diamond

### Unit III Growth techniques and Characterization tools of nanomaterials

Introduction – top-down vs bottom-up technique – Lithographic process and its limitations – Nonlithographic techniques : Sputtering, Chemical Vapour Deposition, Pulsed Laser Deposition, Sol-Gel technique-nucleation and growth processes, Electrodeposition, Scanning Probe Microscopy – General Concept and defining Characteristics of AFM – Electron Microscopy – Transmission Electron Microscopy

### Unit IV Supramolecular Chemistry – I

Introduction to Supramolecular Chemistry – definitions – concepts – molecular forces - covalent bonding, ion – ion, ion – dipole, dipole – dipole, hydrogenbonding, cation –  $\pi$ ,  $\pi$ - $\pi$  interactions, van der Waals forces, hydrophobic and solvent effects – Common motifs in Supramolecular Chemistry – Host/Guest Chemistry, cation, anion and neutral molecule binding. Molecular receptors and design principles.

### **Unit V Supramolecular Chemistry – II**

Principles of molecular association and organization – SAMs, micelles, vesicles and cell membrane –Molecular channels and transport processes - Supramolecular reactivity and catalysis- Molecular devices and Nanotechnology

#### **Books for study**

1. T. Pradeep, NANO: The Essentials: Understanding Nanoscience and Nanotechnology, McGraw Hill Education; 1 edition, 2017)
2. B. S. Murthy, P. Shankar, B. Raj, B. B. Rath, and J. Murday, Textbook of Nanoscience and Nanotechnology, University Press India Private Limited, I edition, 2012.

#### **Books for reference**

1. G.L. Hornyak, J. Dutta, H.F. Tibbals, A.K. Rao, Introduction to Nanoscience, CRC Press, 2008.
2. Mich Wilson, Kamali Kanengara, Geoff Smith, Michelle Simmons and Burkherd Raguk, Nanotechnology Basic Science and Energy Technologies, Overseas press (I), N.D. 2005
3. C.N.R. Rao, A. Muller, A.K. Cheetam (Eds), The Chemistry of Nanomaterials, Vol.1, no 2, Wiley – VCH, Weinheim, 2004.
4. J. W. Steed, J. L. Atwood, “Supramolecular Chemistry”, Wiley, 2000.

#### **Online resources**

1. <http://www.ggu.ac.in/download/Class-Note13/Introduction%20to%20Nanosc.24.10.13.pdf>
2. <https://www.csic.es/en/investigation/research-groups/supramolecular-nanochemistry-and-materials-3>

## **Project Work**

**Programme: M.Sc.,**

**Subject: Chemistry**

**Semester: IV**

**Course: Project work**

**Course Type: Core Paper-I**

**Credits: 5**

**Hours Required: 5 Hrs / week**

**CIA: 40 / CA:60**

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