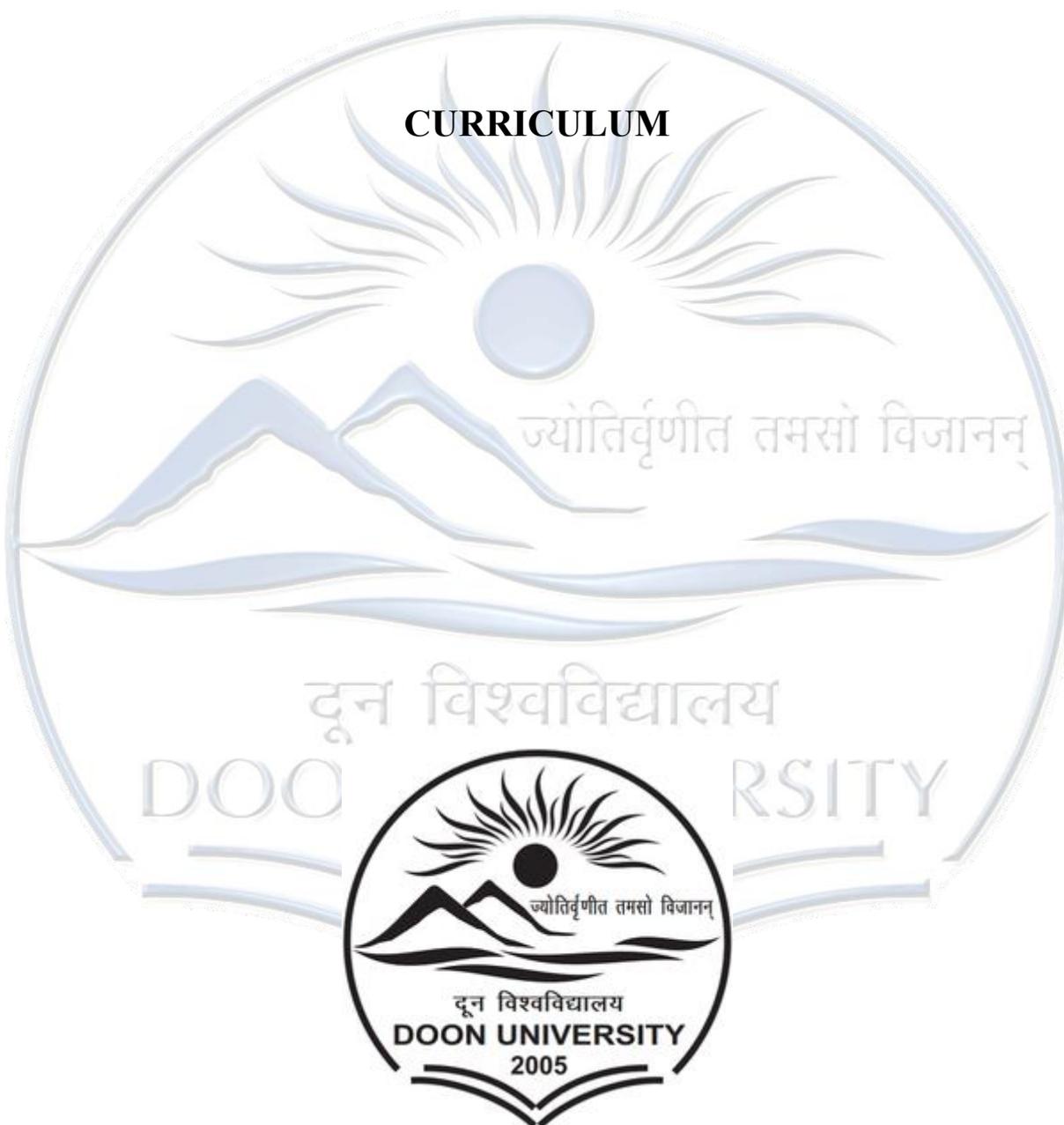


# 02-Years M.Sc. in Chemistry

Applicable July 2025 Onwards



**DEPARTMENT OF CHEMISTRY  
SCHOOL OF PHYSICAL SCIENCES  
DOON UNIVERSITY**

## OBJECTIVES

[1] To impart the key knowledge of chemical sciences and laboratory resources to prepare students for choosing careers in chemistry and related areas with strong scientific depth and temperament.

[2] To prepare students for higher studies in chemistry and the area of their choice.

## PROGRAM OUTCOMES

[PO.1] Students will have a firm foundation in the fundamentals and application of current chemical and basic science including those in Physical, Organic, Inorganic, Analytical and Biochemistry.

[PO.2] Students will be able to seek new knowledge, skills and manage relevant information from various sources.

[PO.3] Students will be trained to work effectively and safely in the laboratory environment independently as well as in teams.

[PO.4] Students will be able to design and carry out scientific experiments as well as accurately draw logical inferences from the results of such experiments.

[PO.5] Students will be able to clearly communicate the results of scientific work in oral, written and ICT formats to both science community and society.

[PO.6] Students will be able to explain why chemistry is an integral activity for addressing social, economic, and environmental problems.

[PO.7] Students will be able to learn and act with integrity and good ethics in their profession and their obligation to society.

[PO.8] Students will be able to demonstrate knowledge and skills in analysing and identifying entrepreneur opportunities.

## COURSE STRUCTURE OF M.Sc. (02 Year PG Program)

### FIRST SEMESTER

Course Type	Course Code	Course Title	L	T	P	C
DSC	CYC-411	Statistical Thermodynamic & Thermochemistry	3	1	0	4
DSC	CYC-412	Organic Molecules: Reactivity And Mechanism	3	1	0	4
DSE/GE		From List of DSE Courses of Chemistry or GE Courses				4
DSE/GE		From List of DSE Courses of Chemistry or GE Courses				4
DSE/GE		From List of DSE Courses of Chemistry or GE Courses				4
SEC	CYS-411	Research Seminar -I	2	0	0	2
Total Credits =						22

### SECOND SEMESTER

Course Type	Course Code	Course Title	L	T	P	C
DSC	CYC-461	Advanced Methods of Chemical Analysis	3	1	0	4
DSC	CYC-462	Organometallic Compounds of Transition Metals in Catalysis and Biology	3	1	0	4
DSE/GE		From List of DSE Courses of Chemistry or GE Courses				4
DSE/GE		From List of DSE Courses of Chemistry or GE Courses				4
DSE/GE		From List of DSE Courses of Chemistry or GE Courses				4
SEC	CYS-461	Research Seminar -II	2	0	0	2
Total Credits =						22

### THIRD SEMESTER

Course Type	Course Code	Course Title	L	T	P	C
DSC	CYS-511	Research Seminar-III	2	0	0	2
DSCP	CYR-511	Dissertation	0	0	20	20
Total Credits =						22

\*DSE: Discipline Specific Elective; These courses are chosen by the students from the list of Discipline Specific Elective (DSE) Courses for 9<sup>th</sup> Semester, given in Table 4.

### FOURTH SEMESTER

Course Type	Course Code	Course Title	L	T	P	C
SEC	CYS-561	Research Seminar-IV	2	0	0	2
DSCP	CYR-561	Dissertation	0	0	20	20
Total Credits =						22

\*DSE: Discipline Specific Elective; These courses are chosen by the students from the list of Discipline Specific Elective (DSE) Courses for 9<sup>th</sup> Semester, given in Table 4.

**[1] Discipline Specific Elective (DSE) Courses in the Area of Inorganic Chemistry For 02 Years M.Sc. Program**

The students will have a liberty to choose Inorganic Chemistry courses from the following list (Table 1) to comply with the credit framework:

<b>Table 1. Discipline Specific Elective (DSE) Courses in the Area of Inorganic Chemistry</b> (for 02 Years M.Sc. Chemistry Program)						
Course Type	Course Code	Course Title	L	T	P	C
DSE	CYE-401	Biological Inorganic Chemistry (Credits: 04)	3	1	0	4
DSE	CYE-402	Structure and Properties of Metal Complexes (Credits: 04)	4	0	0	4
DSE	CYE-403	Frontiers in Bioinorganic Chemistry (Credits: 04)	4	0	0	4
DSE	CYE-404	Frontiers in Inorganic and Bioinorganic Chemistry (Credits: 04)	4	0	0	4
DSE	CYE-405	Inorganic Photochemistry (Credits: 04)	4	0	0	4
DSE	CYE-406	Supramolecular Chemistry (Credits: 04)	4	0	0	4
DSE	CYE-407	Inorganic Solid State Chemistry (Credits: 04)	4	0	0	4
DSE	CYE-471	Inorganic Analysis and Determination Lab (Credits: 04)	0	0	4	4
DSE	CYE-472	Laboratory Synthesis of Inorganic Compounds (Credits: 04)	0	0	4	4

**[2] Discipline Specific Elective (DSE) Courses in the Area of Organic Chemistry For 02 Years M.Sc. Program**

The students will have a liberty to choose Organic Chemistry courses from the following list (Table 2) to comply with the credit framework:

<b>Table 2. Discipline Specific Elective (DSE) Courses in the Area of Organic Chemistry</b> (for 02 Years M.Sc. Chemistry Program)						
Course Type	Course Code	Course Title	L	T	P	C
DSE	CYE-421	Synthetic Organic Chemistry Lab (Credits: 04)	0	0	4	4
DSE	CYE-422	Pericyclic Reactions and Organic Photochemistry (Credits: 04)	3	1	0	4
DSE	CYE-423	Medicinal Chemistry (Credits: 04)	3	1	0	4
DSE	CYE-424	Applied Oxidation, Reduction and C-C Bond Formation Reactions	4	0	0	4

		(Credits: 04)				
DSE	CYE-425	Reagents and Reactions in Organic Chemistry (Credits: 04)	4	0	0	4
DSE	CYE-426	Chemistry of Natural Products (Credits: 04)	3	1	0	4
DSE	CYE-427	Organic Structure Determination (Credits: 04)	3	1	0	4
DSE	CYE-428	One and Two Dimensional NMR Spectroscopic Techniques: Principals and Applications (Credits: 04)	3	1	0	4
DSE	CYE-429	Modern Organic Synthesis Methods (Credits: 04)	3	1	0	4
DSE	CYE-430	Total Organic Synthesis (Credits: 04)	3	1	0	4
DSE	CYE-473	Named Organic Reaction Lab (Credits: 04)	0	0	4	4
DSE	CYE-474	Molecular Organic Synthesis Lab (Credits: 04)	0	0	4	4
DSE	CYE-475	Molecular Purification and Characterization Lab (Credits: 04)	0	0	4	4

### [3] Discipline Specific Elective (DSE) Courses in the Area of Physical Chemistry For 02 Years M.Sc. Program

The students will have a liberty to choose Physical Chemistry courses from the following list (Table 3) to comply with the credit framework:

Course Type	Course Code	Course Title	L	T	P	C
DSE	CYE-441	Physical Chemistry of Surfaces and Interfaces (Credits: 04)	3	1	0	4
DSE	CYE-442	Advanced Surface and Colloidal Chemistry (04 Credits)	4	0	0	4
DSE	CYE-443	Solid State Chemistry (Credits: 04)	3	1	0	4
DSE	CYE-444	Advance Quantum Chemistry (Credits: 04)	3	1	0	4
DSE	CYE-445	Radiation and Photochemistry (Credits: 04)	3	1	0	4
DSE	CYE-446	Advanced Physical Chemistry (Credits: 04)	3	1	0	4
DSE	CYE-447	Biophysical Chemistry (Credits: 04)	3	1	0	4
DSE	CYE-476	Advanced Physical Chemistry Lab-I (Credits: 04)	0	0	4	4

DSE	CYE-477	Advanced Physical Chemistry Lab-II (Credits: 04)	0	0	4	4
DSE	CYE-478	Kinetics and Photochemistry (Credits: 04)	3	1	0	4

#### [4] Discipline Specific Elective (DSE) Courses in the Multidisciplinary / Interdisciplinary Fields of Chemistry For 02 Years M.Sc. Program

The students will have a liberty to choose Physical Chemistry courses from the following list (Table 4) to comply with the credit framework:

<b>Table 4. Discipline Specific Elective (DSE) Courses in the Multidisciplinary / Interdisciplinary Fields of Chemistry (for 02 Years M.Sc. Chemistry Program)</b>						
Course Type	Course Code	Course Title	L	T	P	C
DSE	CYE-461	Methods of Chemical Analysis	3	1	0	4
DSE	CYE-462	Environmental Pollutants and Analysis (Credits: 04)	4	0	0	4
DSE	CYE-463	Macromolecules and Nanomaterials (Credits: 04)	3	1	0	4
DSE	CYE-464	Green Methods of Synthesis (Credits: 04)	3	1	0	4

#### [5] Skill Enhancement Course (SEC) in the Fields of Chemistry For 02 Years M.Sc. Program

The students will have a liberty to choose Physical Chemistry courses from the following list (Table 5) to comply with the credit framework:

<b>Table 5. Discipline Specific Elective (DSE) Courses in the Multidisciplinary / Interdisciplinary Fields of Chemistry (for 02 Years M.Sc. Chemistry Program)</b>						
Course Type	Course Code	Course Title	L	T	P	C
SEC	CYS-411	Research Seminar-I (Credits: 02)	2	0	0	2
SEC	CYS-461	Research Seminar-II (Credits: 02)	2	0	0	2
SEC	CYS-511	Research Seminar-III (Credits: 02)	2	0	0	2
SEC	CYS-561	Research Seminar-IV (Credits: 02)	2	0	0	2
SEC	CYS-403	Laboratory Skills for Physical Chemistry (Credits: 02)	0	0	2	2
SEC	CYS-404	Experimental Skills for Physical Chemistry (Credits: 02)	0	0	2	2
SEC	CYS-405	Physical Chemistry Lab-III (Credits: 02)	0	0	2	2
SEC	CYS-406	Synthetic Skills for Organic Molecules (Credits: 02)	0	0	2	2
SEC	CYS-407	Synthetic Skills for Inorganic	0	0	2	2

		Molecules (Credits: 02)				
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### [6] Dissertation

Traditional teaching, usually based on lectures and tutorials, fosters the idea of instruction-driven learning model where students are passive listeners. However, project-based learning as a different learning paradigm is standing behind constructivism learning theory, where learning from real-world situations is put on the first place.

Students will have to undertake Dissertation (20 Credits) as a Discipline Specific Core (DSC) course at 3<sup>rd</sup> Semester. At 4<sup>th</sup> semester, the students will undertake Dissertation (20 Credits) as a DSC course.

<b>Table 6. Dissertation/Academic Project/Entrepreneurship</b> (for 02 Years M.Sc. Chemistry Program)						
Course Type	Course Code	Course Title	L	T	P	C
DSCP	CYR-511	Dissertation (Credits: 20)	0	0	20	20
DSCP	CYR-561	Dissertation (Credits: 20)	0	0	20	20

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DOON UNIVERSITY  
2005

# CYC-411: Statistical Thermodynamics and Thermochemistry

Discipline Specific Core (DSC) Course for the students of 1<sup>st</sup> Semester of 02 Year M.Sc. Program

<b>Type</b>	:	Core Course
<b>Total Credits</b>	:	04 (Theory: 03 + Tutorial: 01)
<b>Total Hours</b>	:	45 Theory + 15 Tutorial
<b>Lectures</b>	:	03 per week
<b>Tutorial</b>	:	01 per week
<b>Practical</b>	:	0

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## Course Objectives:

[CO.1] To know and understand different statistical approaches used in thermodynamics

[CO.2] To know and understand, theories and concepts related to activation energy and reaction rate

[CO.3] To know and understand thermodynamics of reversible and irreversible electrochemical systems

[CO.4] To know and understand the types of chemical reactions

[CO.5] To know and understand the electron transfer dynamics

## Course Outcomes:

*After completing the course,*

[CO.1] Students will know and understand different statistical approaches used in statistical thermodynamics

[CO.2] Students will know and understand the theories and concepts related to activation energy and reaction rates

[CO.3] Students will know and understand the thermodynamics of reversible and irreversible electrochemical system

[CO.4] Students will know and understand the types of chemical reactions

[CO.5] Students will know and understand the electron transfer dynamics, electron transfer in homogenous and heterogeneous systems

## COURSE CONTENT

### Unit I: Statistical Thermodynamics (15 Hours)

Concept of microstates and ensembles, microcanonical, canonical and grand canonical ensemble, average distribution, partition functions and its relation with thermodynamics properties, Maxwell Boltzmann, Bose-Einstein, Fermi-Dirac statistics, Molecular partition functions, translational, vibrational, and rotational partition functions. Ideal monoatomic and diatomic gases and their thermodynamic properties.

### Unit II: Theories (10 Hours)

Theoretical calculation of energy of activation using potential energy surface diagram, absolute reaction rate theory, comparison between gas phase and solution reactions

### Unit III: Thermodynamics of Ionic Systems (10 Hours)

Thermodynamics of reversible and irreversible electrochemical systems, thermodynamic foundation of theory of ionic interaction and calculation of energy of ionic interaction, interpretation of electrical conductance of electrolytes, thermodynamic treatment of diffusion potential.

### Unit IV: Types of Reactions (5 Hours)

Kinetics of chain reactions, detections of radical and kinetics of HBr, H<sub>2</sub>O<sub>2</sub> reactions, explosion limits, elementary idea of unimolecular reactions, application of following to the reaction kinetics— solvent effect, kinetic isotope effect and salt effect, experimental technique for studying the fast reaction kinetics, kinetics of homogenous and heterogenous catalysis, kinetics of polymerization.

#### Unit V: Electron Transfer Dynamics

(5 Hours)

Electron transfer in homogeneous systems, theory of electron transfer processes, electron tunneling, experimental results, electron transfer in heterogeneous systems, study of kinetics of electrode processes.

#### Suggested Readings

- [1] Seddon, J. M. and Gale, J. D., "*Thermodynamics and Statistical Mechanics*", Royal Society of Chemistry.
- [2] McQuarrie, D. A. and Simon, J. D., "*Physical Chemistry*", Reprint, Viva Student Edition.
- [3] McQuarrie, D. A. "*Statistical Mechanics*", Reprint, Viva Books Pvt. Ltd.
- [4] Atkins, P. W., "*Physical Chemistry*", 7th Ed., ELBS, Oxford University Press.
- [5] Silbey, R.J. and Alberty, R.A. "*Physical Chemistry*", 4th Ed., John Wiley & Sons, Inc., New York.
- [6] West, R., "*Solid State Chemistry and its Applications*" Reprint, Wiley, India.
- [7] Wells, A. F., "*Structural Inorganic Chemistry*", 5th edn., Clarendon Press, Oxford.
- [8] Spaldin, N. "*Magnetic Materials: Fundamentals and Device Applications*", Cambridge University Press.
- [9] Houston, P.L. "*Chemical Kinetics and Reaction Dynamics*", Dover Publications Inc.



1<sup>st</sup> Semester

### **CYC-412: Organic Molecules: Reactivity and Mechanism**

Discipline Specific Core (DSC) Course for the students of 1<sup>st</sup> Semester of 02 Year M.Sc. Program

<b>Type</b>	:	Elective Course
<b>Total Credits</b>	:	04 (Theory: 03 + Tutorial: 01)
<b>Total Hours</b>	:	45 Theory + 15 Tutorial
<b>Lectures</b>	:	03 per week
<b>Tutorial</b>	:	01 per week
<b>Practical</b>	:	0

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### Course Objectives:

- [CO.1] To know and understand the conformations and reactivities of cyclohexane and its derivatives.  
 [CO.2] To know and understand various models to predict stereochemical outcomes of nucleophilic additions to carbonyl compounds.  
 [CO.3] To know and understand the thermodynamics and kinetics aspects of a chemical reactions.  
 [CO.4] To know and understand various methods for elucidation of reaction mechanism.  
 [CO.5] To know and understand different types of catalysis in organic reactions.

### Course Outcomes:

*After completion of the course,*

- [CO.1] Students will understand the reaction mechanisms, reaction coordinate diagrams and Kinetic vs Thermodynamic Control  
 [CO.2] Students will know and understand reaction kinetics, Linear Free Energy Relationships and other related concepts  
 [CO.3] Students will know the thermodynamics and kinetics aspects of a chemical reactions.  
 [CO.4] Students will know and understand various methods for elucidation of reaction mechanism.  
 [CO.5] Students will know and understand different types of catalysis in organic reactions.

## COURSE CONTENT

- Unit 1:** (11 Hours)  
 Introduction to Reaction Mechanisms, Polar Reactions, Radical Reactions, Reaction Coordinate Diagrams, The Hammond Postulate, Kinetic versus Thermodynamic Control, Curtin-Hammett Principle.
- Unit 2:** (12 Hours)  
 Introduction to Reaction Kinetics, Rate Laws, Distinguishing Reaction Mechanisms using Rate Laws, Methods to Monitor a Reaction, The Hammett Equation, Linear Free Energy Relationships (LFER), Hammett Plots for Electronic Effects, Scales used in Hammett Plots, Deviation from Linear Free Energy Relationships (LFER), LFER for Sterics: The Taft Parameters
- Unit 3:** (11 Hours)  
 Solvent Effects, Kinetic Isotope Effect, Primary Kinetic Isotope Effect, Secondary Kinetic Isotope Effect, Heavy Atom Isotope Effects, Equilibrium Isotope Effects, Isotope Labelling, Trapping Intermediates, Common Intermediates.
- Unit 4:** (11 Hours)  
 Catalysis, Specific Catalysis, General Catalysis, Enzyme Catalysis, Electrophilic Catalysis and Other Types of Catalysis

### Suggested Readings:

- [1] F. A. Carey and R. I. Sundberg, Advanced Organic Chemistry, Part A, 3rd edition, Plenum Press, 1990.
- [2] E. V. Anslyn, D. A. Dougherty Modern Physical Organic Chemistry.
- [3] Peter Sykes, A guidebook to mechanisms in Organic Chemistry.



2<sup>nd</sup> Semester

### **CYC-461: Advanced Methods of Chemical Analysis**

Discipline Specific Core (DSC) Course for the students of 2<sup>nd</sup> Semester of 02 Year M.Sc. Program

<b>Type</b>	:	Elective Course
<b>Total Credits</b>	:	04 (Theory: 03 + Tutorial: 01)
<b>Total Hours</b>	:	45 Theory + 15 Tutorial
<b>Lectures</b>	:	03 per week
<b>Tutorial</b>	:	01 per week
<b>Practical</b>	:	0

### Course Objectives:

[CO.1] To know and understand the principles and instrumentation of vibrational spectroscopy, electron spin resonance spectroscopy, NMR spectroscopy, Mossbauer spectroscopy, X-ray photoelectron spectroscopy (XPS) and X-ray diffraction (XRD) techniques.

[CO.2] To learn how to use such techniques in chemical analysis.

### Course Objectives:

*After completion of the course,*

[CO.1] Student(s) will know and understand the principles and instrumentation of vibrational spectroscopy, electron spin resonance spectroscopy, NMR spectroscopy, Mossbauer spectroscopy, X-ray photoelectron spectroscopy (XPS) and X-ray diffraction (XRD) techniques.

[CO.2] Student(s) will learn how to use such techniques in chemical analysis.

## COURSE CONTENT

### Unit I: Vibrational Spectroscopy

Symmetry and shapes of AB<sub>2</sub>, AB<sub>3</sub>, AB<sub>4</sub>, AB<sub>5</sub> and AB<sub>6</sub>, modes of bonding of ambidentate ligands, ethylenediamine and diketonate complexes, application of resonance Raman Spectroscopy particularly for the study of active sites of metalloproteins as myoglobin and haemoglobin.

### Unit II: Electron Spin Resonance Spectroscopy

Principle, presentation of the spectrum, hyperfine coupling, hyperfine splitting in various structures, factors affecting magnitude of g, zero field splitting and Kramer's degeneracy, applications to transition metal complexes having one and more than one unpaired electron, applications to inorganic free radicals, study of electron exchange reactions.

### Unit III: NMR spectroscopy:

Principle and Instrumentation.

### Unit IV: Mossbauer Spectroscopy

Basic principles, spectral display, isomer shift, factors affecting the magnitude of isomer shift, quadrupole and magnetic hyperfine interaction, applications of technique to the study of bonding and structure of Fe<sup>2+</sup>, Fe<sup>3+</sup>; Sn<sup>2+</sup> and Sn<sup>4+</sup> compounds; detection of oxidation stated nature of M-L bond.

### Unit V:

Principles and Applications of XRD and XPS.

### Suggested Readings

[1] Drago, R.S., "*Physical Methods in Inorganic Chemistry*", Reinhold Publishing Corp., East West Press.

[2] Graybeal, J. D., "*Molecular Spectroscopy*", McCarraw-Hill, 1988.

[3] Slichter. C. P., "*Principles of Magnetic Resonance*", Springer Verlag, 1981.

[4] Banweil, C.N. and McCash, E.L.M., "*Fundamentals of Molecular Spectroscopy*", 4<sup>th</sup> Ed. McGraw-Hill. 1999.

2<sup>nd</sup> Semester

## CYC-462: Organometallic Compounds of Transition Metals in Catalysis & Biology

Discipline Specific Core (DSC) Course for the students of 2<sup>nd</sup> Semester of 02 Year M.Sc. Program

<b>Type</b>	:	Core Course
<b>Total Credits</b>	:	04 (Theory: 03 + Tutorial: 01)
<b>Total Hours</b>	:	45 Theory + 15 Tutorial
<b>Lectures</b>	:	03 per week
<b>Tutorial</b>	:	01 per week
<b>Practical</b>	:	0

### Course Objectives:

- [CO.1] To know and understand different types of metathesis reactions and their catalysis  
 [CO.2] To know and understand the oligomerization and polymerization reactions of olefins  
 [CO.3] To know and understand the homo polymerization and copolymerization reactions  
 [CO.4] To know and understand bioorganometallic chemistry, metal ions in biology, metalloenzymes, Coenzyme B12, nitrogenase, urease and other relevant metalloenzymes.

### Course Outcomes:

*After completing the course,*

- [CO.1] Students will know and understand different types of metathesis reactions and their catalysis  
 [CO.2] Students will know and understand the oligomerization and polymerization reactions  
 [CO.3] Students will know and understand the homo polymerization and copolymerization  
 [CO.4] Students will know and understand bioorganometallic chemistry, metal ions in biology, metalloenzymes, Coenzyme B12, nitrogenase, urease and other relevant metalloenzymes.

## COURSE CONTENT

### Unit 1:

Introduction, Reppe synthesis, Reppe Reactions, Metallative and Conventional Reppe and Metathesis Reaction, Origin of Olefin Metathesis, Development of Metathesis, classifications, Mechanistic approaches of Metathesis Reaction, Catalysts Development Aspect of Olefin Metathesis, Cross-Metathesis, Ring Opening Metathesis and Ring Closing Metathesis, Alkyne metathesis reactions: history, classifications, mechanism, Alkene Alkyne Metathesis, Ring Closing Eneyne Metathesis.

### Unit 2:

Olefin oligomerization reactions, Oligomerization reactions of alkenes and alkynes, Olefin polymerization reactions: polyethylene, polypropylene, Ziegler-Natta catalyst, Other catalysts in olefin polymerization reactions,

### Unit 3:

Homo polymerization with functionalized olefins, cycloolefins, diolefins, Copolymerization with functionalized olefins, cycloolefins, diolefins, Non-Group 4 catalysts

### Unit 4:

Bioorganometallic Chemistry, metal ions in biology, metalloenzymes, Coenzyme B12, nitrogenase, urease and other relevant metalloenzymes.

### Suggested Readings:

- [1] Elschenbroich (Organometallics)  
 [2] Crabtree (The Organometallic Chemistry of the Transition Metals)  
 Discipline Specific Elective (DSE) Course in the Area of Inorganic Chemistry For 02 Years M.Sc. Program

## CYE-401: Biological Inorganic Chemistry

(For the students of 02 Year PG Program in Chemistry)

<b>Type</b>	:	Elective Course
<b>Total Credits</b>	:	04 (Theory: 03 + Tutorial: 01)
<b>Total Hours</b>	:	45 Theory + 15 Tutorial
<b>Lectures</b>	:	03 per week
<b>Tutorial</b>	:	01 per week
<b>Practical</b>	:	0

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### Course Objectives:

[CO.1] To know and understand important role of metal ions in biology, health, diseases and medicine.

[Co.2] To know and understand the inorganic aspects of life processes and biological processes from the viewpoint of the coordination chemistry of metal ions.

[CO.3] To know and understand the involvement of the selected metal ions in cellular and subcellular functions.

### Course Outcomes:

*After completion of the course,*

[CO.1] Student(s) will know and understand the important role of metal ions in biology, health, diseases and medicine.

[CO.2] Student(s) will know and understand the magnetic properties of transition metal complexes

[CO.3] Student(s) will know and understand the involvement of the selected metal ions in cellular and subcellular functions.

## COURSE CONTENT

### Unit 1:

Outline of metal ions in biology, Natural and biological ligands for essential metal ions

### Unit 2:

Physical methods to study metal ions biological systems, Assimilation pathways, transport, storage and homeostasis of biogenic metal ions, Ion channels and pumps involving sodium and potassium ions, Magnesium ions for phosphate metabolism and cellular signaling using calcium ions, Iron ions in life processes: dioxygen management

### Unit 3:

Biochemistry of copper ions, Enzymes containing zinc ions: Action of Lewis acid, Biological actions of manganese, cobalt and nickel ions

### Unit 4:

Nonmetallic species in biology, Metal ions in brain and medicine

### Suggested Readings

[1] Biocoordination Chemistry, D E Fenton, OUP, 2002

[2] Principles of Bioinorganic Chemistry, S J Lippard and, J M Berg, USB, California, 1994

[3] Biological Inorganic Chemistry, R R Crichton, Elsevier, 2012

Discipline Specific Elective (DSE) Course in the Area of Inorganic Chemistry For 02 Years M.Sc. Program

## CYE-402: Structure and Properties of Metal Complexes

		(For the students of 02 Year PG Program in Chemistry)
<b>Type</b>	:	Elective Course
<b>Total Credits</b>	:	04 (Theory: 4 + Practical: 0)
<b>Total Hours</b>	:	60 Theory + 0 Practicals
<b>Lectures</b>	:	04 per week
<b>Tutorial</b>	:	0
<b>Practical</b>	:	0

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### Course Objectives:

- [CO.1] To know and understand the stereochemistry and bonding in inorganic compounds of main group elements, metal-ligand bonding, molecular orbital theory, metal-ligand equilibria in solution, electronic spectra of coordination compounds, and
- [CO.2] To know and understand the magnetic properties of transition metal complexes

### Course Outcomes:

*After completion of the course,*

- [CO.1] Student(s) will know and understand the stereochemistry and bonding in inorganic compounds of main group elements, metal-ligand bonding, molecular orbital theory, metal-ligand equilibria in solution, electronic spectra of coordination compounds, and
- [CO.2] Student(s) will know and understand the magnetic properties of transition metal complexes

## COURSE CONTENT

### Unit I: Stereochemistry and bonding in main group compounds

VSEPR theory, Walsh diagrams (tri- and penta-atomic molecules) d<sub>r</sub> - p<sub>r</sub> bonds, bent rule and energetics of hybridization, some simple reactions of covalently bonded molecules, stereoisomerism in inorganic complexes, isomerism arising out of ligand and ligand conformation, chirality and nomenclature of chiral complexes.

### Unit II: Metal-ligand bonding and molecular orbital theory (MOT)

Limitations of crystal field theory, d-orbitals splitting in linear, trigonal, octahedral, square planar, tetrahedral and square pyramidal complexes, Jahn-Teller distortion, nephelauxetic series, composition of ligand group orbitals, molecular orbital diagrams of octahedral, tetrahedral, square planar complexes including both  $\sigma$  and  $\pi$  bonding.

### Unit III: Metal-ligand equilibria in solution

Stepwise and overall formation constants and their interaction, trends in stepwise constants, factors affecting the stability of metal complexes with references to the nature of metal ion and ligand, chelate effect and its thermodynamic origin, determination of binary formation constants by pH-metry and spectrophotometry.

### Unit IV: Electronic spectra of coordination compounds

Spectroscopic ground states, correlation and spin-orbit coupling in free ions for 1<sup>st</sup> series of transition metals, Orgel and Tanabe Sugano diagrams for transition metal complexes (d<sup>n</sup> - d<sup>n</sup> states), calculation of Dq, B and  $\beta$  parameters, effect of distortion on d-orbital energy levels.

### Unit V: Magnetic properties of transition metal complexes

Fundamental equations in molecular magnetism, magnetic susceptibility and magnetic moment, diamagnetic and paramagnetic behaviour of transition metal complexes, spin-orbit coupling effects (L-

S coupling and j-j coupling), orbital angular moment and its quenching in octahedral and tetrahedral complexes, temperature independent paramagnetism (TIP) of complexes, spin cross over, ferromagnetic, anti-ferromagnetic, ferrimagnetic behaviour of transition metal compounds, effect of temperature on their magnetic properties.

### Suggested Readings

- [1] Cotton, F. A., Wilkinson, G., Murillo, C. A. and Bochmann, M., "*Advanced Inorganic Chemistry*", 6th Ed., John Wiley & Sons, **1999**.
- [2] Douglas, B. E., McDaniel, D. H. and Alexander, J. J., "*Concepts and Models in Inorganic Chemistry*", 3rd Ed., John Wiley & Sons, **2001**.
- [3] Figgis, B. N., and Hitchman, M. A., "*Ligand Field Theory and Its Applications*", Wiley Eastern Ltd., **1999**.
- [4] Huheey, J. E., Keiter, E. A. and Keiter, R. L., "*Inorganic Chemistry Principle of Structure and Reactivity*", 4th Ed, Pearson Education, Inc., **2003**.
- [5] Atkins, P., Overton, T., Rourke, J., Mark, W. and Armstrong, F., "*Shriver and Atkins' Inorganic Chemistry*", 4th Ed, Oxford university press, **2009**.



## **CYE-403: Frontiers in Bioinorganic Chemistry**

(For the students of 02 Year PG Program in Chemistry)

<b>Type</b>	:	Elective Course
<b>Total Credits</b>	:	04 (Theory: 4 + Practical: 0)
<b>Total Hours</b>	:	60 Theory + 0 Practicals
<b>Lectures</b>	:	04 per week
<b>Tutorial</b>	:	0
<b>Practical</b>	:	0

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### **Course Objectives:**

[CO.1] To know and understand the concepts of bioinorganic chemistry including homeostatic mechanism, metal ion transport, assembly of metalloproteins, role of molybdenum and tungsten in biology, and iron in biosystem

[CO.2] To know and understand the role of metal ions in context of specific diseases, and biominerals

### **Course Outcomes:**

*After completion of the course,*

[CO.1] Student(s) will be able to know and understand the concepts of bioinorganic chemistry including homeostatic mechanism, metal ion transport, assembly of metalloproteins, role of molybdenum and tungsten in biology, and iron in biosystem

[CO.2] Student(s) will understand the role of metal ions in context of specific diseases, and biominerals

## **COURSE CONTENT**

### **Unit I: Homeostatic mechanism**

Cellular components and pathways in the context of metal ions, homeostatic mechanism in cell - prokaryotes to eukaryotes to human. Evolutionary pathway metals, metallocofactors and prosthetic groups.

### **Unit II: Metal ion transport and assembly of metalloproteins:**

Details of the metal transport in Yeast and in higher organisms, proteins involved in uptake and efflux, assembly of metals in protein, photoactivation, heme synthesis, covalent and non-covalent interactions of heme with protein, assembly of heme in heme proteins- cytochrome c vs cytochrome b5, heme chaperoning and role of CCME, identification of a protein as heme protein, heme oxygenase, reconstitution of hemeproteins with modified heme/other cofactors and their application in biocatalysis and electron transfer.

### **Unit III: Molybdenum and Tungsten in Biology**

Hyperthermophilic and thermophilic bacteria, Mo and W containing enzymes, mechanism of catalytic activity- nitrogenase, sulfite oxidase, nitrate reductase, acetylene hydratase, xanthine oxidase, DMSO reductase, structural and functional modeling of Mo and W sites and their applications as biocatalysis.

### **Unit IV: Iron in Biosystem**

Non-heme-iron-sulphur proteins, other non-heme iron proteins-lipoxygenase and its implication in cancer research, nitrile hydratase and its application to industry, structural and functional modeling of heme and non-heme metal-sites and their applications in biochemistry, heme-catalytic mechanism of nitric oxide synthase and heme oxygenase.

### **Unit V: Metal Ions and Diseases**

Role in Alzheimer's disease- aggregation of proteins, role of copper, zinc and iron, application of radiochemistry for the identification of metal ions, metal binding in prion protein-binding of

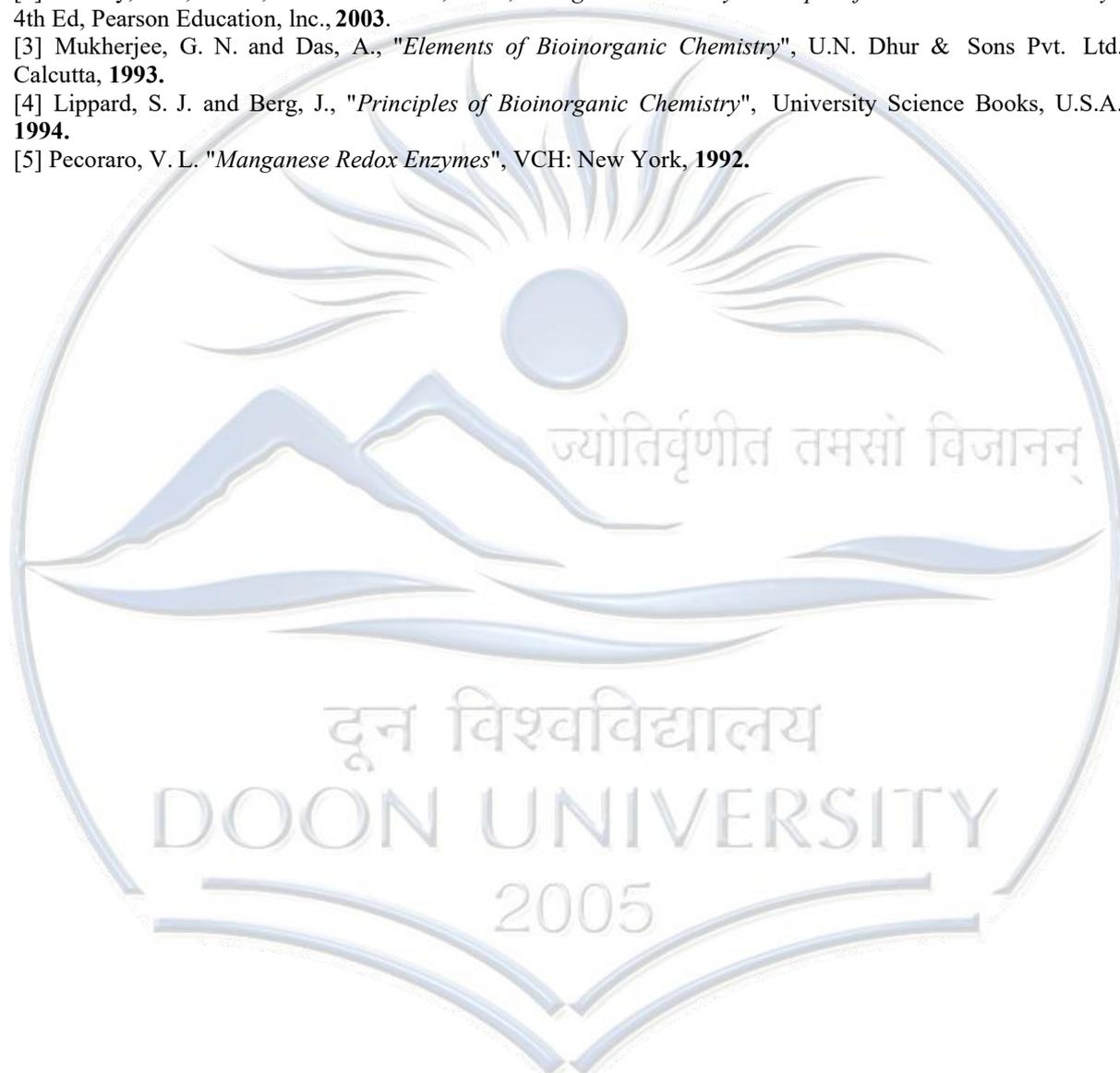
copper and manganese, manganese- occupational exposure, manganese toxicity, effect on calcium channel, proteomics of manganese toxicity, inorganic NO-donor and their applications.

#### **Unit VI: Biomineralization**

Biomineralization in the context of bone, teeth and mollusk cells, application into materials science and biomimetic engineering, bioorganometallic chemistry- introduction and applications.

#### **Suggested Readings**

- [1] Cotton, F. A., Wilkinson, G., Murillo, C. A. and Bochmann, M., "*Advanced Inorganic Chemistry*", 6th Ed., John Wiley & Sons, **1999**.
- [2] Huheey, J. E., Keiter, E. A. and Keiter, R. L., "*Inorganic Chemistry Principle of Structure and Reactivity*", 4th Ed, Pearson Education, Inc., **2003**.
- [3] Mukherjee, G. N. and Das, A., "*Elements of Bioinorganic Chemistry*", U.N. Dhur & Sons Pvt. Ltd., Calcutta, **1993**.
- [4] Lippard, S. J. and Berg, J., "*Principles of Bioinorganic Chemistry*", University Science Books, U.S.A., **1994**.
- [5] Pecoraro, V. L. "*Manganese Redox Enzymes*", VCH: New York, **1992**.



## **CYE-404: Frontiers in Inorganic and Bioinorganic Chemistry**

(For the students of 02 Year PG Program in Chemistry)

<b>Type</b>	:	Elective Course
<b>Total Credits</b>	:	04 (Theory: 4 + Practical: 0)
<b>Total Hours</b>	:	60 Theory + 0 Practicals
<b>Lectures</b>	:	04 per week
<b>Tutorial</b>	:	0
<b>Practical</b>	:	0

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### **Course Objectives:**

[CO.1] To know and understand the reaction mechanisms of transition metal complexes, and electron transfer reactions

[CO.2] To know and understand the photochemistry of metal complexes, and concepts of inorganic biochemistry

[CO.3] To know and understand the chemical toxicity and metallotherapy

### **Course Outcomes:**

*After completion of the course,*

[CO.1] Student(s) will know and understand the reaction mechanisms of transition metal complexes, and electron transfer reactions

[CO.2] Student(s) will know and understand the photochemistry of metal complexes, and concepts of inorganic biochemistry

[CO.3] Student(s) will know and understand the chemical toxicity and metallotherapy

## **COURSE CONTENT**

### **Unit 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 planer complexes, the trans effect.

### **Unit II: Electron Transfer Reactions**

Outer- and inner-sphere mechanisms, factors affecting electron transfer reaction rates, cross reactions and Marcus- Hush theory, solvated electron.

### **Unit III: Photochemistry of Metal Complexes**

Introduction to inorganic photochemistry, photochemically excited states and excited state processes for transition metal complexes, photochemical reactions of coordination compounds, types of photochemical reactions in transition metal complexes substitution, decomposition, rearrangement and redox reactions, applications of photochemical inorganic reactions in synthesis, catalysts, biological processes and in lasers.

### **Unit IV: Inorganic biochemistry:**

Metalloproteins and enzymes – role of metal ions in active sites, structure and functions of metalloproteins and enzymes containing Mg, Ca, V, Mn, Fe, Co, Ni, Cu and Zn ions, detailed structure and mechanistic studies of the following—Mn- photosystem-II, catalase, pseudocatalase, oxygen carriers, haemoglobin, myoglobin, non-porphyrin oxygen carriers, hemerythrin, hemocyanin, Fe-ribonucleotide reductase, cytochrome c oxidases, cytochrome P-450s, hydrogenase, nitrogen fixation,

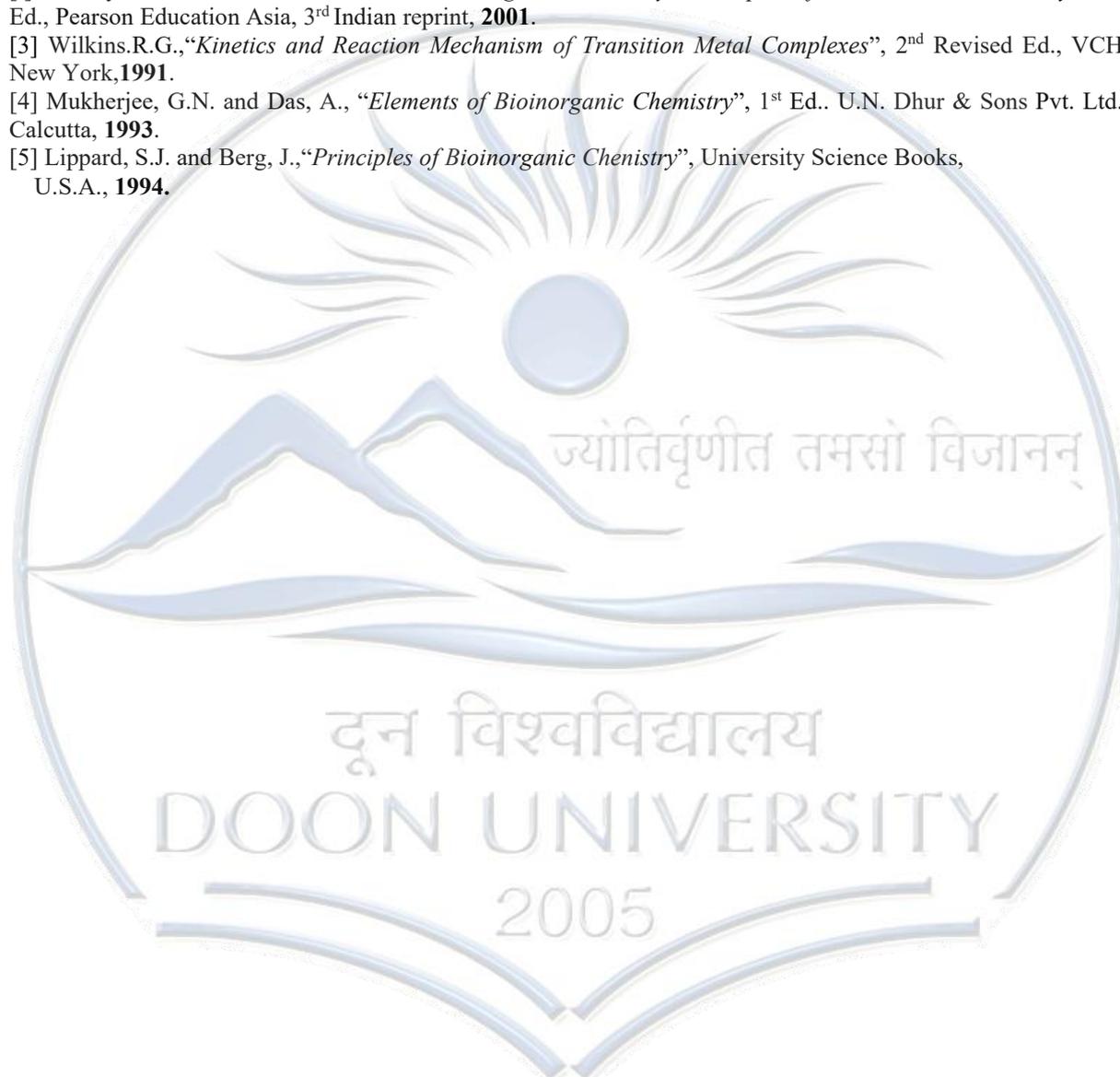
Cu-blue copper protein, tyrosinase, galactose oxidase, superoxide dismutases, Zn-carbonicanhydrase, carboxypeptidase, alcohol dehydrogenase, biological importance of Vitamin B12 and coenzyme.

#### **Unit V: Chemical toxicity and Metallotherapy:**

Toxic chemicals in the environment, toxic effects of arsenic, cadmium, lead, mercury, carbon monoxide, cyanide and other carcinogens, metal containing drugs in therapy, interaction of heavy metal ions with DNA, DNA cleavage, structure-activity relationship and mode of action.

#### **Suggested Readings**

- [1] Huheey, J.E., Keiter, E. and Keiter, R., "*Inorganic Chemistry: Principles of Structure and Reactivity*", 4th Ed., Pearson Education Asia, 3<sup>rd</sup> Indian reprint, **2001**.
- [3] Wilkins.R.G., "*Kinetics and Reaction Mechanism of Transition Metal Complexes*", 2<sup>nd</sup> Revised Ed., VCH, New York, **1991**.
- [4] Mukherjee, G.N. and Das, A., "*Elements of Bioinorganic Chemistry*", 1<sup>st</sup> Ed.. U.N. Dhur & Sons Pvt. Ltd., Calcutta, **1993**.
- [5] Lippard, S.J. and Berg, J., "*Principles of Bioinorganic Chenistry*", University Science Books, U.S.A., **1994**.



## **CYE-405: Inorganic Photochemistry**

(For the students of 02 Year PG Program in Chemistry)

<b>Type</b>	:	Elective Course
<b>Total Credits</b>	:	04 (Theory: 4 + Practical: 0)
<b>Total Hours</b>	:	60 Theory + 0 Practicals
<b>Lectures</b>	:	04 per week
<b>Tutorial</b>	:	0
<b>Practical</b>	:	0

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### **Course Objectives:**

[CO.1] To know and understand the fundamentals of photochemistry

[CO.2] To know and understand the properties of the excited states, excited states of metal complexes

[CO.3] To know and understand the excited states of metal complexes, and ligand-field photochemistry

[CO.4] To know and understand the redox reactions by excited metal complexes, and metal complexes as sensitizers

### **Course Outcomes:**

*After completion of the course,*

[CO.1] Students will know and understand the fundamentals of photochemistry, the properties of the excited states, and excited states of metal complexes

[CO.2] Students will know and understand the excited states of metal complexes, and ligand-field photochemistry

[CO.3] Students will know and understand the redox reactions by excited metal complexes, and metal complexes as sensitizers

## **COURSE CONTENT**

### **Unit I: Basics of photochemistry:**

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

### **Unit II: Properties of excited states:**

Structure, dipole moment, acid-base strengths, reactivity, photochemical kinetics-calculation of rates of radiative processes, bimolecular deactivation - quenching.

### **Unit III: Excited states of metal complexes:**

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

### **Unit IV: Ligand field photochemistry:**

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

### **Unit V: Redox reactions by excited metal complexes:**

Energy transfer under conditions of weak interaction and strong interaction-exciplex formation; conditions of the excited states to be useful as redox reactants, excited electron transfer, metal complexes as attractive candidates ( ,2'-bipyridine and I,10-phenanthroline complexes), illustration of reducing and oxidizing character of Ru(II)-bipyridinal complex, comparison with

Fe(bipy)<sub>3</sub>; role of orbit coupling- life time of these complexes, application of redox processes of electronically excited states for catalytic purposes, transformation of low energy reactants into high energy products, chemical energy into light.

#### **Unit VI: Metal complex sensitizers:**

Metal complex sensitizer, electron relay, metal colloid systems, semiconductor supported metal or oxide systems, water photolysis, nitrogen fixation.

#### **Suggested Readings**

- [1] *Concepts of Inorganic Photochemistry*, A. W. Adamson and P. D. Fleischauer, Wiley.
- [2] *Inorganic Photochemistry*. J. Chem. Educ., vol. 60, no. 10, 1983.
- [3] *Progress in Inorganic Chemistry*, vol. 30 ed.S. J. Lippard. Wiley.
- [4] *Coord. Chem. Rev.*, vol. 39, 121, 131; 1975, 15,321; 1990, 97,313.
- [5] *Photochemistry of Coordination Compounds*, V. Balzani and V. Carassiti, Academic Press.
- [6] *Elements of Inorganic Photochemistry*. G. J. Ferraudi, Wiley.



## **CYE-406: Supramolecular Chemistry**

(For the students of 02 Year PG Program in Chemistry)

<b>Type</b>	:	Elective Course
<b>Total Credits</b>	:	04 (Theory: 4 + Practical: 0)
<b>Total Hours</b>	:	60 Theory + 0 Practicals
<b>Lectures</b>	:	04 per week
<b>Tutorial</b>	:	0
<b>Practical</b>	:	0

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### **Course Objectives:**

- [CO.1] To know and understand the fundamentals of supramolecular chemistry
- [CO.2] To know and understand the role of supramolecular chemistry in biological processes
- [CO.3] To learn how to synthesize the supramolecules
- [CO.4] To know and understand the methods and their use in supramolecular chemistry

### **Course Outcomes:**

*After completion of the course,*

- [CO.1] Student(s) will know and understand the fundamentals of supramolecular chemistry.
- [CO.2] Student(s) will know and understand the role of supramolecular chemistry in biological processes.
- [CO.3] Student(s) will have the skills to synthesize the supramolecules.
- [CO.4] Student(s) will know and understand the methods and their use in supramolecular chemistry.

## **COURSE CONTENT**

### **Unit I: Fundamentals of Supramolecular Chemistry** (15 hours)

Introductory remarks and relevance of study. The original meaning of “supramolecular Chemistry” and how it has changed over the years to include various systems of study. Various intermolecular interactions and the meaning of molecular recognition, Concepts of positive and negative cooperativity, Thermodynamic treatment of molecular recognition.

### **Unit II: Supramolecular Synthons** (15 hours)

Introduction of supramolecular synthons, synthesis of macrocycles, thermodynamic and kinetic template effects. Macrocyclic effects and stability, crown ethers and lariat crown ethers, Macrocyclic effects, thermodynamic and kinetic stability of complexes. Calixarenes and the art of molecular basket making, conformational flexibility of calixarenes at room temperature and their binding characteristics. Hybrids of calixarenes and their uses, Cucurbiturils of different sizes and their characteristics. Use of cucurbiturils in chemical reactions. Cyclodextrins and their structural characteristics as supramolecular reaction vessels.

### **Unit III: Macrobicyclic Cryptands, Cyclophanes, Cryptophanes and Spherands** (15 hours)

Strategy and methodology for Synthesis, Rigidity and conformational lability of cryptands, layer effects, Synthesis of cryptands and cryptates of cations and anions and the cryptate effects, Mononuclear and multinuclear cryptates of transition metal ions and their uses in homogeneous catalysis, Cyclophanes and cryptophanes, Inclusion of non-polar organic molecules and other properties, Spherands and their synthesis and metal binding properties.

#### Unit IV: Dendrimers, Interlocked Structures and Metal Helicates

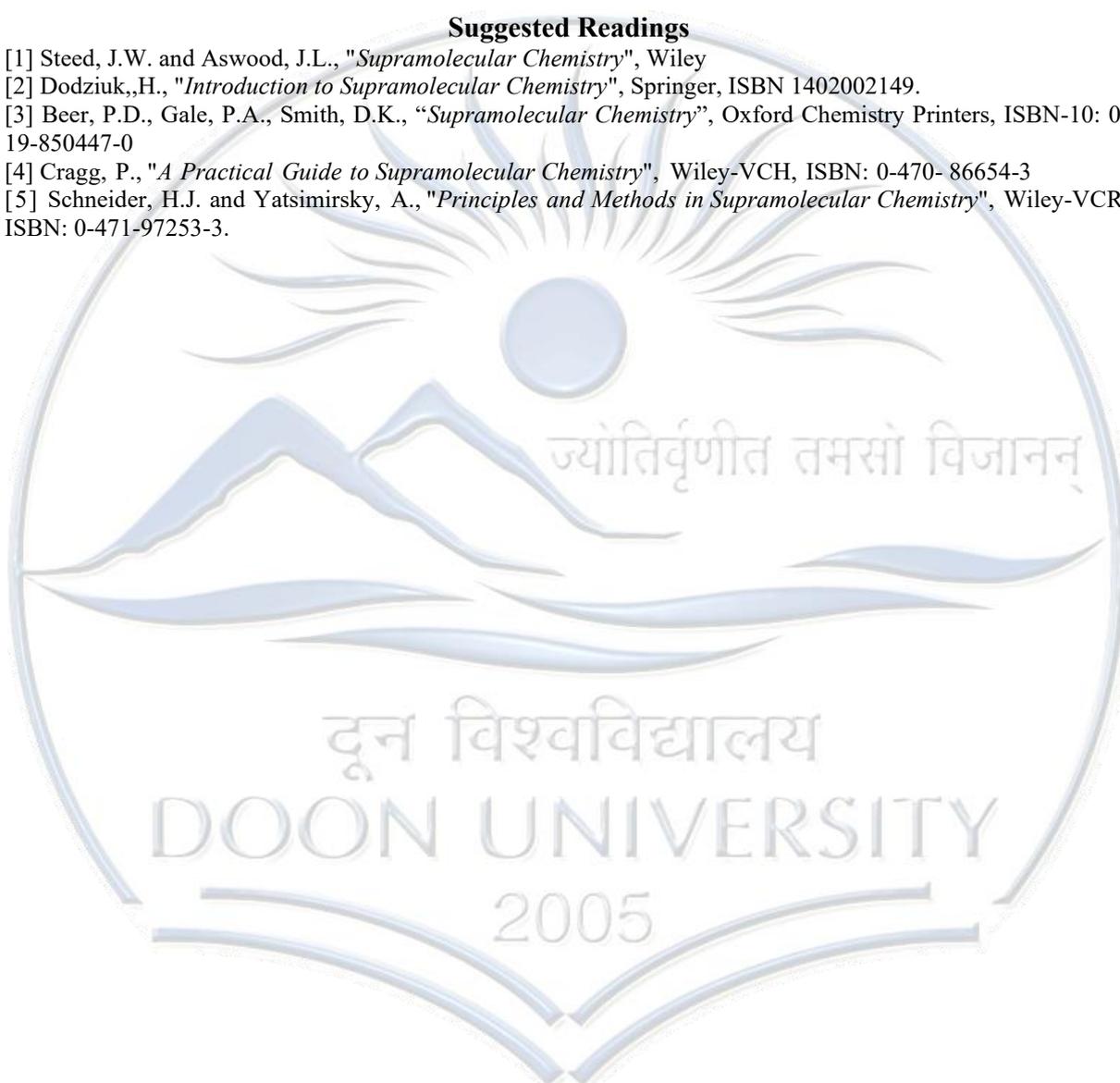
(15 hours)

Dendrimers and their structural characteristics, Synthesis of dendrimers by divergent and convergent methods, Binding properties of dendrimers and mimicry of metalloproteins' active sites, catalysis.

Interlocked structures of different designs: pseudo-rotaxanes, rotaxanes, molecular shuttle, Metal helicates, catenanes and catenates, trefoil knots. Synthesis of these complex structures via metal templating and p-p stacking interactions.

#### Suggested Readings

- [1] Steed, J.W. and Aswood, J.L., "*Supramolecular Chemistry*", Wiley
- [2] Dodziuk, H., "*Introduction to Supramolecular Chemistry*", Springer, ISBN 1402002149.
- [3] Beer, P.D., Gale, P.A., Smith, D.K., "*Supramolecular Chemistry*", Oxford Chemistry Printers, ISBN-10: 0-19-850447-0
- [4] Cragg, P., "*A Practical Guide to Supramolecular Chemistry*", Wiley-VCH, ISBN: 0-470- 86654-3
- [5] Schneider, H.J. and Yatsimirsky, A., "*Principles and Methods in Supramolecular Chemistry*", Wiley-VCR, ISBN: 0-471-97253-3.



## **CYE-407: Inorganic Solid-state Chemistry**

(For the students of 02 Year PG Program in Chemistry)

<b>Type</b>	: Elective Course
<b>Total Credits</b>	: 04 (Theory: 4 + Practical: 0)
<b>Total Hours</b>	: 60 Theory + 0 Practicals
<b>Lectures</b>	: 04 per week
<b>Tutorial</b>	: 0
<b>Practical</b>	: 0

### Course Objectives:

[CO.1] To know and understand the crystal structures of inorganic compounds, and defect structures

[CO.2] To learn how to synthesize solid state materials.

[CO.3] To know and understand amorphous inorganic materials, intercalation chemistry.

[CO.4] To know the use of physical methods in the structural characterization of metal complexes.

### Course Outcomes:

*After completion of the course,*

[CO.1] Students will know and understand the crystal structures of inorganic compounds, and defect structures.

[CO.2] Students will know how to synthesize solid state materials

[CO.3] Students will know and understand amorphous inorganic materials, intercalation chemistry

[CO.4] Students will know and understand the use of physical methods in the structural characterization of metal complexes.

## **COURSE CONTENT**

### **Unit I: Crystal structure of inorganic compounds**

Overview of close packing, packing efficiency, interstitial sites, limiting radius ratios, method of determination of ionic radii. Ionic crystals containing two or three different elements– FeO, ZnO, CdS, fluorite, antiferite, nickel-arsenide,  $\text{CaC}_2$ ,  $\text{CdI}_2$  and  $\text{TiO}_2$ ,  $\text{FeTiO}_3$ ,  $\text{MgAl}_2\text{O}_4$ ,  $\text{Fe}_2\text{NiO}_4$ , garnets,  $\text{BaTiO}_3$  and  $\text{KNiF}_3$ . Non-ionic crystals– SiC,  $(\text{BN})_x$ , giant molecules, layer structures, crystals composed of discrete molecules.

### **Unit II: Defect structures**

Thermodynamic defects and their consequences, solid electrolytes, non-stoichiometric compounds, F-centers and applications of defects in non-stoichiometric compounds.

### **Unit III: Methods to synthesize solid-state materials**

Ceramic method, solid-state reaction and its kinetics, hydrothermal, sol-gel, co-precipitation (precursor), vapour phase transport methods. Different methods to grow single crystals.

### **Unit IV: Amorphous Inorganic Materials**

Glasses, refractories, materials obtained from organometallic chemical vapour deposition (MOCVD). New materials: Conducting polymers, carbon nanotubes, carbon nanorods and fullerenes. Electronic materials: Insulating, semiconducting and superconducting materials, ferroelectrics and dielectrics.

### **Unit V: Intercalation chemistry**

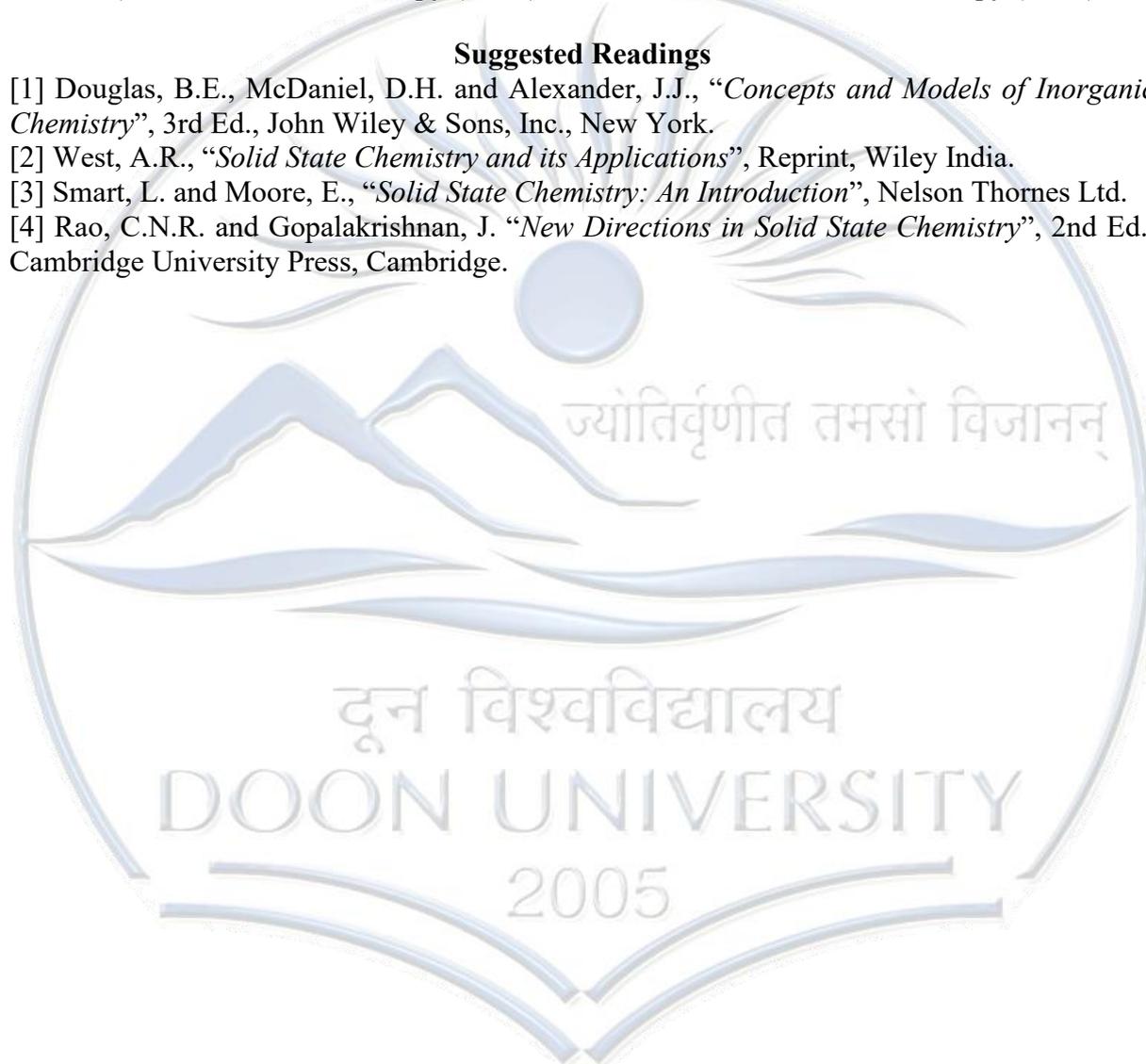
Introduction, intercalation reactions in graphite, layered double hydroxides, layered sulfides, applications of intercalation chemistry. Mesoporous materials and their catalytic applications: Various types of mesoporous materials (oxides, sulphides), tailoring of pore size, applications of mesoporous materials in heterogeneous catalysis.

#### **Unit VI: Structural Characterization of Metal Complexes by Physical Methods**

Extended X-ray absorption spectroscopic (EXAFS), X-ray photoelectron spectroscopic (XPS), X-ray absorption near edge spectroscopic (XANES), electron spin spectrometric (ESR), electron spectroscopy for chemical analysis (ESCA) studies, solid state NMR, HMBC, HMQC, Mössbauer spectroscopic studies of metal complexes, thermal methods (TG, DTA and DSC), atomic force microscopy (AFM) and transmission electron microscopy (TEM).

#### **Suggested Readings**

- [1] Douglas, B.E., McDaniel, D.H. and Alexander, J.J., “*Concepts and Models of Inorganic Chemistry*”, 3rd Ed., John Wiley & Sons, Inc., New York.
- [2] West, A.R., “*Solid State Chemistry and its Applications*”, Reprint, Wiley India.
- [3] Smart, L. and Moore, E., “*Solid State Chemistry: An Introduction*”, Nelson Thornes Ltd.
- [4] Rao, C.N.R. and Gopalakrishnan, J. “*New Directions in Solid State Chemistry*”, 2nd Ed., Cambridge University Press, Cambridge.



## CYE-471: Inorganic Analysis and Determination Lab

(For the students of 02 Year PG Program in Chemistry)

Type	:	Elective Course
Total Credits	:	04 (Theory: 0 + Practical: 4)
Total Hours	:	00 Theory + 60 Practicals
Lectures	:	0
Tutorial	:	0
Practical	:	60 per week

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### Course Objectives:

[CO.1] To introduce the principles of electronic spectroscopy of coordination compounds and verify the spectrochemical series using nickel complexes along with spectrophotometric estimation.

[CO.2] To provide practical knowledge of complexometric titration using EDTA for the determination of hardness of water.

[CO.3] To introduce the principles of electronic spectroscopy of coordination compounds and verify the spectrochemical series using nickel complexes along with spectrophotometric estimation.

[CO.4] To introduce students to instrumental analytical techniques such as Atomic Absorption Spectroscopy (AAS) for determination of metals in alloy samples.

### Course Outcomes:

*After completion of the course,*

[CO.1] Students will know the principles of semi-micro qualitative analysis and identify cations including interfering radicals in unknown samples using systematic analysis.

[CO.2] Students Analyze metal ions using combined gravimetric and volumetric techniques, including the estimation of Fe(II) and Ca(II).

[CO.3] Interpret electronic spectra of coordination complexes and verify the spectrochemical series using complexes of Ni(II), and estimate nickel spectrophotometrically.

[CO.4] Determine the concentration of alkali metals (Na and K) in soil samples using flame photometry and understand its analytical significance.

### COURSE CONTENT

[1] Semi-micro qualitative analysis involving 6 radicals including interfering radicals.

[2] Determination of hardness of water by complexometric titration with EDTA.

[3] Gravimetric estimation of nickel using dimethyl glyoxime.

[4] Determination of metal ions by gravimetric-cum-volumetric analysis: Fe(II) gravimetrically and Ca(II) volumetrically.

[5] Determination of Cu(II) gravimetrically and Zn(II) volumetrically

[6] Experiment related to gravimetric determination and separation of two metal ions in a binary mixture.

[7] Comparison of electronic spectra of  $[\text{Ni}(\text{H}_2\text{O})_6]^{2+}$ ,  $[\text{Ni}(\text{NH}_3)_6]^{2+}$  and  $[\text{Ni}(\text{en})_3]^{2+}$  and qualitative verification of the spectrochemical series, and quantitative estimation of nickel by spectrophotometry.

[8] Simultaneous spectrophotometric determination of concentration of  $\text{KMnO}_4$  and  $\text{K}_2\text{Cr}_2\text{O}_7$  in a given mixture.

[9] Determination of Na, K in a soil sample by flame photometry.

[10] Determination of metal in alloy samples by AAS.

*Note: Minimum eight experiments must be done and some would require more two-three turns.*

### Suggested Readings

- [1] Mendham, J., Denney, R.C., Barnes J.D. and Thomas M.J.," Vogel's Text Book of Quantitative Chemical Analysis", 6th Ed., ELBS Longman Group UK Ltd. (2004)
- [2] Vogel's Qualitative Inorganic Analysis, Revised by G. Svehla. Marr & Rockett "Inorganic Preparations"
- [3] Srivastava T.N. and Kamboj P.C., "Analytical Chemistry", Vishal Publications.
- [4] Marr & Rockett "Practical Inorganic Chemistry"



## CYE-472: Laboratory Synthesis of Inorganic Compounds

(For the students of 02 Year PG Program in Chemistry)

Type	:	Elective Course
Total Credits	:	04 (Theory: 0 + Practical: 4)
Total Hours	:	00 Theory + 60 Practicals
Lectures	:	0
Tutorial	:	0
Practical	:	60 per week

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### Course Objectives:

[CO.1] To develop practical understanding of the synthesis of coordination compounds, particularly copper, cobalt, nickel, iron, and manganese complexes.

[CO.2] To introduce students to spectrophotometric techniques for studying coordination complexes and for the quantitative estimation of metal ions.

[CO.3] To develop experimental skills in synthesis, purification, and characterization of coordination compounds using techniques such as metal estimation, spectroscopy, magnetic moment determination, and photochemical studies.

### Course Outcomes:

*After completion of the course,*

[CO.1] Synthesize various coordination compounds of transition metals and understand their preparation methods.

[CO.2] Record and interpret electronic spectra of metal complexes and arrange ligands according to their field strength in the spectrochemical series.

[CO.3] Characterize synthesized coordination compounds using metal content determination, spectroscopic techniques, magnetic moment measurements, and photochemical studies.

[CO.4] Synthesize and analyze different transition metal complexes and organometallic/coordination compounds, and determine their metal content quantitatively.

### COURSE CONTENT

[1] Synthesis and spectrophotometric study of copper complexes: (i) Synthesis of bis(salicylaldehyde)copper(II) and cis-bis (glycinato)copper(II) (ii) Record the spectra bis(salicylaldehyde)copper(II) and cis- bis (glycinato)copper(II), and (iii) Record spectra of  $\text{Cu}^{2+}$  in water,  $\text{NH}_3$ , ethylene diamine and glycine, and arrange the ligands in order of increasing field strength and (iv) Quantitative estimation of copper by spectrophotometry or some other available technique.

[2] (i) Study of the complex formation between Fe(III) and thiocyanate/salicylic acid/sulphosalicylic acid or between Ni(II) and o-phenanthroline, and (ii) Spectrophotometric determination of formation of constant of the complex (Job's method and molar ratio method).

[3] Synthesis of potassium tris(oxalate)aluminate, potassium tris(oxalate)chromate and potassium tris(oxalate)ferrate, and their characterization by metal determination, some spectroscopic methods, magnetic moment determination, and photochemical behaviour of iron complex.

[4] Synthesis and characterization of  $[\text{Co}(\text{en})_3]\text{Cl}_3$ . Separation of its optical isomers and determination of their optical rotation by using a polarimeter.

[5] Extraction of Fe using 8-hydroxyquinoline,

[6] Preparation of bis-(diisopropylamine)chlorophosphate,  $(i\text{-PrN})_2\text{PCl}$

- [7] Preparation of bis-chloro bis-triphenylphosphine nickel(II)
- [8] Preparation of cis and trans-dichloro bis (ethylenediamine)cobalt(III) chloride
- [9] Synthesis and characterization of co-crystals of 5,7,7,12,14,14-hexamethyl-1,4,8,11-tetraazacyclotetradeca-4,1,1-diene with perchloric acid Synthesis of pentaamminechlorocobalt(III) chloride
- [10] Synthesis of following coordination compound(s) and metal content determination: (i)  $[\text{Cu}(\text{NH}_3)_4 \cdot \text{H}_2\text{O}]\text{SO}_4$ , (ii)  $[\text{Fe}(\text{acac})_3]$ , (iii)  $[\text{Mn}(\text{acac})_3]$ , (iv)  $\text{Mn C}_2\text{O}_4 \cdot 3\text{H}_2\text{O}$ .

*Note: Minimum eight experiments must be done and some would require more two-three turns.*

#### Suggested Readings

- [1] Mendham, J., Denney, R.C., Barnes J.D. & Thomas M.J., "Vogel's Text Book of Quantitative Chemical Analysis", 66 Ed., ELBS Longman Group UK Ltd.
- [2] "Vogel's Qualitative Inorganic Analysis", Revised by G. Svehla.
- [3] Marr & Rockett "Inorganic Preparations"
- [4] Gerard Srivastava T. N. & Kamboj P.C., "Analytical Chemistry". Vishal Publications. 2000
- [5] Marr & Rockett "Practical Inorganic Chemistry"



## CYE-421: Synthetic Organic Chemistry Lab

(For the students of 02 Year PG Program in Chemistry)

Type	:	Elective Course
Total Credits	:	04 (Theory: 0 + Practical: 4)
Total Hours	:	0 Theory + 120 Practicals
Lectures	:	0
Tutorial	:	0
Practical	:	04 per week

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### Course Objectives:

- [CO.1] To learn how to carry out organic reactions such as bromination reaction, nitration, reaction, Cannizzaro reaction, aldol condensation, oxidation reaction, Sandmeyer reaction, Knoevenagel condensation, Wittig reaction, Diels Alder reaction, Friedel Crafts reaction, Fisher indole synthesis etc
- [CO.2] To learn how to synthesize and purify the organic compounds.

### Course Outcomes:

*After completion of the course,*

- [CO.1] Student(s) will have the skills to carry out organic reactions such as bromination reaction, nitration, reaction, Cannizzaro reaction, aldol condensation, oxidation reaction, Sandmeyer reaction, Knoevenagel condensation, Wittig reaction, Diels Alder reaction, Friedel Crafts reaction, Fisher indole synthesis etc
- [CO.2] Student(s) will have the skills to synthesize and purify the organic compounds.

## COURSE CONTENT

- [1] Separation of organic mixtures by TLC and PTLC.
- [2] Synthesis of derivatives for carbonyl, amino and active methylene compounds.
- [3] Nitration of methyl benzoate
- [4] Bromination of acetanilide.
- [5] Preparation of *p*-nitroaniline of acetanilide
- [6] Cannizzaro reaction of an aromatic Aldehyde (*p*-nitrobenzaldehyde).
- [7] Aldol condensation (benzaldehyde + acetone or cinnamaldehyde + acetone)
- [8] Oxidation of hydroquinone to *p*-benzoquinone.
- [9] Oxidation of benzoin to benzyl.
- [10] Conversion of benzyl to quinoxaline.
- [11] Reduction of Camphor.
- [12] Synthesis of 2-iodobenzoic acid by Sandmeyer reaction.
- [13] Synthesis of binaphthol by green reaction.
- [14] Knoevenagel condensation between aldehyde (4-diethylaminobenzaldehyde) and malonic acid, cyanoacetic acid or malononitrile.
- [15] Friedel-Crafts reaction: synthesis of 1,4-*di-tert-butyl*-2,5-dimethoxy benzene.
- [16] Diels-Alder reaction between anthracene and maleic anhydride.
- [17] Preparation and purification of *cis*- and *trans*-stilbenes by Wittig reaction.
- [18] Preparation of pyridium dichromate and its uses in oxidation of benzyl alcohol.
- [19] Synthesis of  $\omega$ -nitrostyrene from an aromatic aldehyde and nitromethane
- [20] Synthesis of chalcone from an aromatic aldehyde and acetophenone.
- [21] Extraction of oils from ground nuts using Soxhlet apparatus

[22] Synthesis of  $\alpha$ -bromo cinnamic acid or phenyl acetylene from benzaldehyde, (formation of cinnamic acid, bromination and elimination reactions).

[23] Preparation of *meso*-stilbene dibromide and its conversion to diphenylacetylene.

[24] Fisher indole synthesis.

*Note: Some experiments would require two-three turns, and minimum ten experiments must be done.*

#### Suggested Readings

[1] Arthur, I. V., "Quantitative Organic Analysis," Pearson.

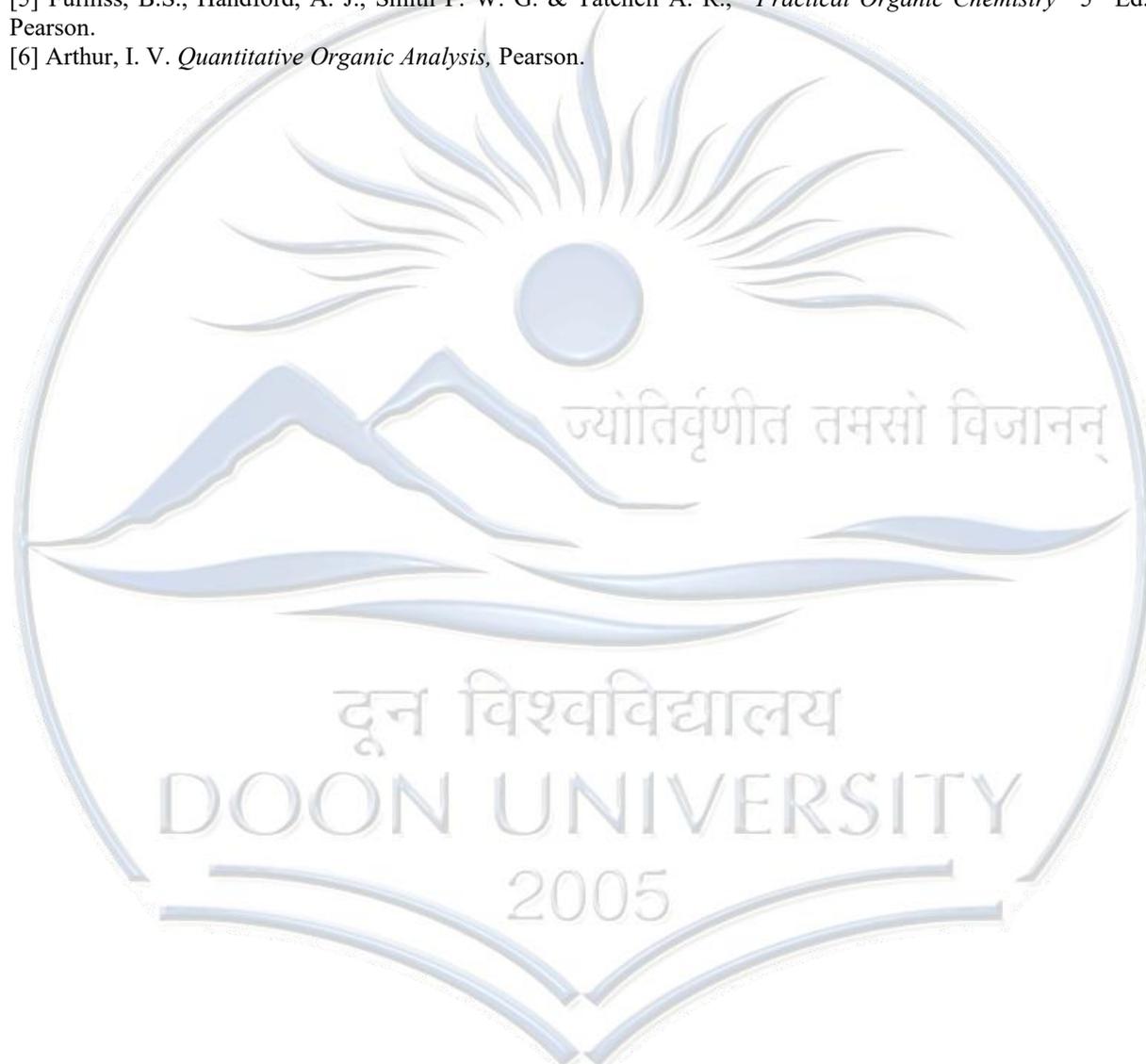
[2] Furniss, B.S., Handford, A. J., Smith P. W. G. & Tatchell A. R., "Vogel's Text Book of Practical Organic Chemistry" 5<sup>th</sup> Ed. Longman (1996).

[3] Leonard J., Lygo B. & Procter G., "Advanced Practical Organic Chemistry", Champan and Hall. (1995)

[4] Mann, F. G. & Saunders, B.C. "Practical Organic Chemistry", Pearson. (2009)

[5] Furniss, B.S., Handford, A. J., Smith P. W. G. & Tatchell A. R., "Practical Organic Chemistry" 5<sup>th</sup> Ed., Pearson.

[6] Arthur, I. V. *Quantitative Organic Analysis*, Pearson.



## **CYE-422: Pericyclic Reactions and Organic Photochemistry**

(For the students of 02 Year PG Program in Chemistry)

<b>Type</b>	:	Elective Course
<b>Total Credits</b>	:	04 (Theory: 3 +Tutorial: 1)
<b>Total Hours</b>	:	45 Theory + 15 Tutorial
<b>Lectures</b>	:	03 per week
<b>Tutorial</b>	:	01 per week
<b>Practical</b>	:	0

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### **Course Objectives:**

[CO.1] To know and understand the classifications of pericyclic reactions, molecular orbital symmetry and frontier molecular orbital concepts.

[CO.2] To know and understand different electrocyclic reactions with even numbers of electron participation.

[CO.3] To know and understand sigmatropic rearrangements and their types in pericyclic reactions.

[CO.4] To know and understand photochemical reactions in organic chemistry.

### **Course Outcomes:**

After completion of this course, the students will know and understand the classifications of pericyclic reactions, molecular orbital symmetry, frontier molecular orbital concepts, different electrocyclic reactions with even numbers of electron participation, Diels-Alder reaction, sigmatropic rearrangements and photochemical reactions in organic chemistry.

## **COURSE CONTENT**

### **Unit I: Basic Concepts and Electrocyclic Reactions**

Activation of chemical reactions, Thermal and photochemical methods, MOs of polyene and their symmetry properties and methods of analyzing pericyclic reactions, Introduction to electrocyclic reactions and Woodward Hoffmann rules, Examples of 3, 4 and 5 membered ring systems (2e and 4e systems), Examples of 6 and larger ring systems (6e and more)

### **Unit II: Cycloaddition Reactions**

Introduction and Woodward Hoffmann rules, [2+2] cycloadditions, ketene cycloadditions, Diels-Alder reaction, Woodward Hoffmann rule for Diels-Alder reaction, Regiochemistry and Stereochemistry aspects of Diels-Alder Reaction, Synthetic applications of Diels-Alder Reaction, Diels Alder reaction of Hetero diene and dienophile, Lewis acid mediated Diels Alder Reaction, Asymmetric Diels-Alder reaction.

1,3-Dipolar cycloaddition reactions, [4 pi + 4pi], [4 pi + 6 pi] and higher order cycloaddition reactions

### **Unit III: Sigmatropic Rearrangement, Chelotropic Reactions and Ene Reaction**

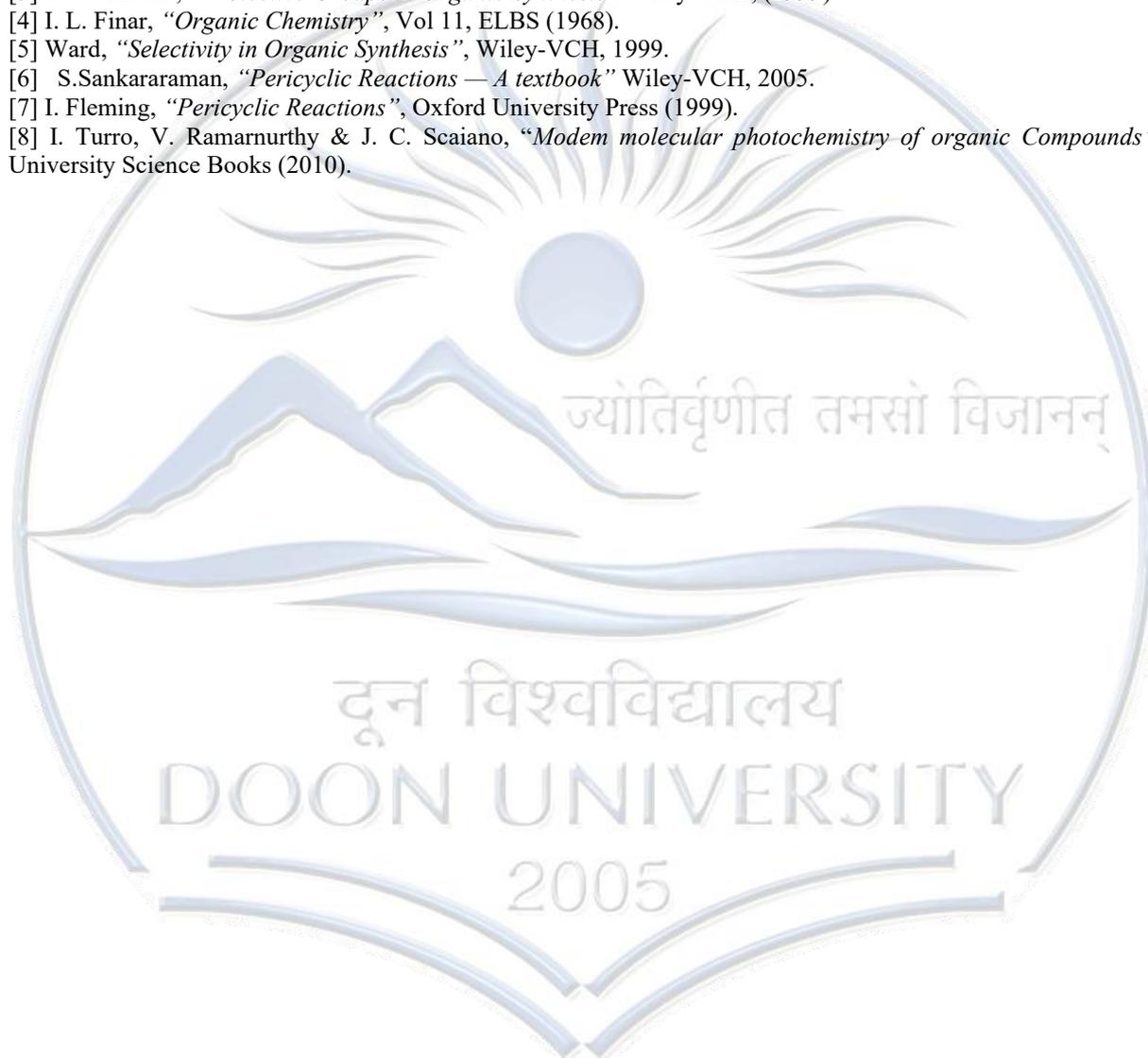
Introduction and [1,3] migrations, [1,5] H and C migrations and Cope rearrangement, Oxy Cope and Claisen Rearrangement, [2,3] sigmatropic shifts and higher order rearrangements, Wittig rearrangement and higher order Sigmatropic shifts, Chelotropic reactions - introduction, SO<sub>2</sub> extrusion reactions, Problems on sigmatropic reactions, Problems on chelotropic reactions, The Ene Reaction

## Unit IV: Organic Photochemistry

Introduction to organic photochemistry, Photochemistry of alkenes, cis-trans isomerization, Photochemistry of carbonyl compounds, Norrish type 1 and 2 reactions, Photochemistry of carbonyl compounds, enone and dienone photochemistry, Photochemistry of Nitrogen compounds, Photochemistry of aromatic compounds, Photoinduced electron transfer reactions.

### Suggested Readings

- [1] I. Fleming & John Wiley *"Frontier Orbital and Organic Chemical Reactions"* 1976.
- [2] W. Carruthers *"Some modern Methods of Organic Synthesis"* Cambridge University Press, (1990).
- [3] T.W. Greene, *"Protective Groups in Organic Synthesis"* Wiley-VCH, (1999)
- [4] I. L. Finar, *"Organic Chemistry"*, Vol 11, ELBS (1968).
- [5] Ward, *"Selectivity in Organic Synthesis"*, Wiley-VCH, 1999.
- [6] S.Sankararaman, *"Pericyclic Reactions — A textbook"* Wiley-VCH, 2005.
- [7] I. Fleming, *"Pericyclic Reactions"*, Oxford University Press (1999).
- [8] I. Turro, V. Ramamurthy & J. C. Scaiano, *"Modern molecular photochemistry of organic Compounds"*, University Science Books (2010).



## CYE-423: Medicinal Chemistry

(For the students of 02 Year PG Program in Chemistry)

Type	:	Elective Course
Total Credits	:	04 (Theory: 3 +Tutorial: 1)
Total Hours	:	45 Theory + 15 Tutorial
Lectures	:	03 per week
Tutorial	:	01 per week
Practical	:	0

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### Course Objectives:

[CO.1] To know and understand the drugs, and intermolecular interactions

[CO.2] To know and understand the drug targets including proteins, enzymes and receptors, their structures and functions

[CO.3] To know and understand the concepts of pharmacokinetic and pharmacodynamics, the enzymes as drug targets, receptors as drug targets, and nucleic acids as drug targets

[CO.4] To know and understand the drug discovery, design, development, identification of the structure–activity relationships (SARs), and the pharmacophore in the drug design, and the ways to improve target interactions (pharmacodynamics) and improve pharmacokinetic properties.

[CO.5] To know and understand the preclinical trials and significance of patent on the drug

### Course Outcomes:

*After completion of the course,*

[CO.1] Student(s) will know and understand the drugs, and intermolecular interactions.

[CO.2] Student(s) will know and understand the drug targets including proteins, enzymes and receptors, their structures and functions.

[CO.3] Student(s) will know and understand the concepts of pharmacokinetic and pharmacodynamics, the enzymes as drug targets, receptors as drug targets, and nucleic acids as drug targets.

[CO.4] Student(s) will know and understand the drug discovery, design, development, identification of the structure–activity relationships (SARs), and the pharmacophore in the drug design, and the ways to improve target interactions (pharmacodynamics) and improve pharmacokinetic properties.

[CO.5] Student(s) will understand the preclinical trials and significance of patent on the drug.

## COURSE CONTENT

### Unit I: Overview of Drugs and Drug Targets

Overview of drugs and drug targets, structure of a cell, intermolecular binding forces, classification of drugs, principles of enzyme structure, catalysis and inhibition in drug discovery: Enzyme mechanisms overview; enzyme catalysis and inhibition in drug discovery; reversible and irreversible inhibitors; transition-state inhibitors; case studies, Receptors function and ligand binding interactions; Ion channel receptors; kinase-linked receptors; G-Protein coupled receptors, drug-receptor interaction; dose-response curves; case studies

### Unit II: Nucleic Acids

Nucleic acids structure and function; DNA Interactive agents and chemotherapy: DNA binding agents; intercalation and alkylation; DNA strand breakers; case studies,

### Unit II: Synthetic Methods in Medicinal Chemistry

Combinatorial and parallel synthesis, solid phase techniques, mix and split method in combinatorial synthesis, dynamic combinatorial synthesis, solid phase synthesis, diversity-oriented synthesis,

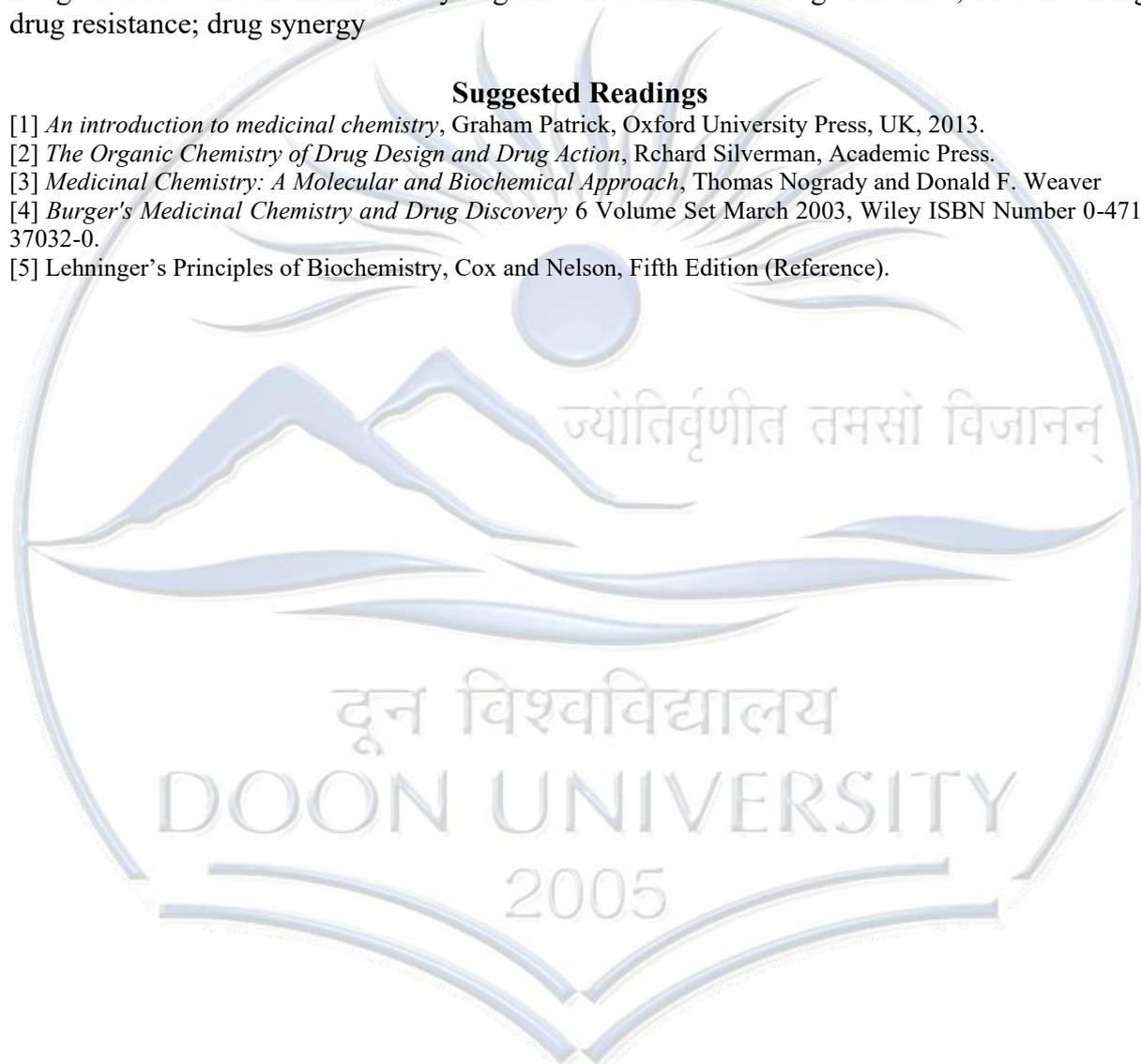
Lead discovery, Bioassays, drug targets, Lead Modification, optimization, pharmacophore, homology, bioisostere, chain branching, Electronic effects, Lipophilicity, Structure-Activity Relationships, Quantitative-structure activity relationships (QSAR).

#### **Unit IV: Drug Metabolism and Pharmacology**

Drug metabolism and pharmacology: Analytical methods in metabolism; Phase I and Phase II transformations, Absorption, distribution, metabolism and excretion (ADME), bioavailability; pre-clinical and clinical development, therapeutic index and therapeutic window, Prodrugs and drug delivery systems: Use of prodrug systems; prodrugs for stability, solubility and slow release; overview of drug delivery, Drug resistance mechanisms and synergism: Mechanisms of drug resistance; circumventing drug resistance; drug synergy

#### **Suggested Readings**

- [1] *An introduction to medicinal chemistry*, Graham Patrick, Oxford University Press, UK, 2013.
- [2] *The Organic Chemistry of Drug Design and Drug Action*, Richard Silverman, Academic Press.
- [3] *Medicinal Chemistry: A Molecular and Biochemical Approach*, Thomas Nogrady and Donald F. Weaver
- [4] *Burger's Medicinal Chemistry and Drug Discovery* 6 Volume Set March 2003, Wiley ISBN Number 0-471-37032-0.
- [5] *Lehninger's Principles of Biochemistry*, Cox and Nelson, Fifth Edition (Reference).



## CYE-424: Applied Oxidation, Reduction and C-C Bond Formation Reactions

(For the students of 02 Year PG Program in Chemistry)

Type	:	Elective Course
Total Credits	:	04 (Theory: 4 + Practical: 0)
Total Hours	:	60 Theory + 0 Practicals
Lectures	:	04 per week
Tutorial	:	0
Practical	:	0

### Course Objectives:

- [CO.1] To know and understand the reagents which are used in organic reactions.
- [CO.2] To know and understand the methods for oxidation reactions.
- [CO.3] To know and understand various types of reducing reactions and reagents.
- [CO.4] To know and understand asymmetric synthesis.
- [CO.5] To know and understand various C–C bond forming reactions.
- [CO.6] To know and understand organometallic compounds which may be used for C-C bond forming reactions.

### Course Outcomes:

*After completion of the course,*

- [CO.1] Students will know and understand the reagents which are used in organic reactions.
- [CO.2] Students will know and understand the methods for oxidation reactions.
- [CO.3] Students will know and understand various types of reducing reactions and reagents.
- [CO.4] Students will know and understand asymmetric synthesis.
- [CO.5] Students will know and understand various C–C bond forming reactions.
- [CO.6] Students will know and understand organometallic compounds which may be used for C-C bond forming reactions.

## COURSE CONTENT

### Unit 1: Oxidation Reactions

Chemistry of Organoselenium Compounds, SeO<sub>2</sub> as the Reagent for Oxidation Reactions, Application of SeO<sub>2</sub> in the Oxidation of Ketones and Sulfoxide-Sulfenate Rearrangement (Mislow-Evans rearrangement) with mechanistic and stereochemical aspects as well as Applications in Synthetic Organic Chemistry, Saegusa-Ito oxidation, 1,2-Ketone transpositions, Shapiro reaction and Dauben-Michno Rearrangement (a case of 1,3-enone transposition), Dess-Martin periodinane oxidation, Iodoxybenzoic acid (IBX) based oxidations, Prevost reaction, use of Fetizon's reagent (Ag<sub>2</sub>CO<sub>3</sub>/Celite) along with mechanistic and stereochemical aspects of the reactions, Ruthenium tetraoxide (RuO<sub>4</sub>) and RuCl<sub>3</sub>/NaIO<sub>4</sub> for Oxidation Reactions, TPAP (Tetra-n-propylammonium perruthenate) for oxidation reactions, Tamao-Fleming oxidation reactions with mechanistic and synthetic aspects, Oxidation reactions through the use of DMDO (Dimethyl Dioxirane) with mechanistic aspects, Oxaziridine Mediated Alpha-Hydroxylations of Ketones, Barton and Related Reactions (Oxidation at Unfunctionalized carbons) with their applications in synthesis, TEMPO (2,2,6,6-tetramethylpiperidine-1-oxyl) for Oxidation Reactions, Pinnick Oxidation and Pseudomonas Putida Mediated Oxidation Reactions.

### Unit 2: Reduction Reactions and Reagents

Reduction reactions using sodium borohydride (NaBH<sub>4</sub>), Lithium Aluminium Hydride (LiAlH<sub>4</sub>), Diisobutylaluminium Hydride (DIBAL-H), Red-Al, Zn(BH<sub>4</sub>)<sub>2</sub>, LiBHET<sub>3</sub> (superhydride) & L & K-selectrides, LS/KS selectrides, NaCNBH<sub>3</sub> and Luche Reductions.

Reductions through Dissolving Metals (Na, K, Mg), McMurry Coupling using Titanium(0) with mechanistic and stereochemistry related aspects, Metal mediated reductions of *Alpha*, *Beta*-Unsaturated Ketones.

Reductions using Silanes ( $R_3SiH$ ) such as Polymethylhydrosiloxanes (PMHS), Barton-McCombie Deoxygenation, and *n*- $Bu_3SnH$  (tributyltinhydride) for radical based reduction reactions and C-C bond forming reactions.

### Unit 3: Asymmetric Synthesis

Introduction, Sharpless Asymmetric Epoxidation (Mechanism, Stereochemistry and Kinetic Resolution), Applications of Chiral 2,3-epoxy Alcohols, Katsuki-Jacobsen Epoxidation with Mechanism and Stereochemistry of Reactions, Sharpless Asymmetric Dihydroxylation with Mechanism and Stereochemistry, Asymmetric Hydrogenations and Reductions using Chiral Catalysts having Rhodium (Rh) and Ruthenium (Ru), and Asymmetric Reduction with Oxazaborolidines.

### Unit 4: C-C Bond Formations

Introduction to Enolate, Enamine and Enol Silyl Ether Based Chemistry, SAMP and RAMP as the Auxiliaries in the Asymmetric Alkylation, Asymmetric C-C bond formation using Oppolzer's camphorsultams, directed Aldol reactions, the applications of boron and silicon enolates in Aldol chemistry, Evans' Oxazolidinone chemistry in context of C-C bond formations.

Ireland-Claisen rearrangement, Enolate Geometry & Stereochemical Outcome, Claisen rearrangements, carbon-carbon bond forming reactions with Evans' Oxazolidinones, Ireland-Claisen Rearrangement with Influence of Enolate Geometry on the Stereochemical Outcome, Claisen Rearrangements, Aromatic Claisen rearrangement, Johnson-Claisen Rearrangement and Eschenmoser-Claisen rearrangement and synthetic Bellus-Claisen rearrangement, Aza-Claisen rearrangement, Thia-Claisen rearrangement, Chen-Mapp rearrangements, Zwitterionic-Claisen Rearrangement, Overmann rearrangement, Bamford-Stevens and Shapiro reactions and synthetic applications.

### Unit 5: Organometallic Compounds for C-C Bond Forming Reactions,

Mechanistic and Stereochemical Aspects of Allylindium compounds, Allyltin compounds, and Allylsilanes along with their applications in synthesis, Mechanistic and Stereochemical Aspects of the Reactions of Vinylsilanes and their Applications in Synthetic Organic Chemistry, Peterson Olefination, Mechanistic & Stereochemical Aspects of Simmons-Smith Cyclopropanation reactions and its applications in synthetic organic chemistry

#### Suggested Readings

- [1] Carey, F. A. and Sundberg, R.I., "*Advanced organic Chemistry, Part B: Reaction and Synthesis*", 5<sup>th</sup> Ed. Springer
- [2] Anslyn, E. V. and Dougherty, D. A., "*Modern Physical Organic Chemistry*", University Science Books.
- [3] Clayden, J., Greeves, N. and Warren, S., "*Organic Chemistry*", Oxford University Press.
- [4] Smith, M.B., "*Organic Synthesis*", 3s Ed., Academic Press.
- [5] Bruckner, R., "*Organic Mechanisms: Reactions, Stereochemistry and Synthesis*", Springer.

## **CYE-425: Reagents and Reactions in Organic Chemistry**

(For the students of 02 Year PG Program in Chemistry)

<b>Type</b>	:	Elective Course
<b>Total Credits</b>	:	04 (Theory: 4 + Practical: 0)
<b>Total Hours</b>	:	60 Theory + 0 Practicals
<b>Lectures</b>	:	04 per week
<b>Tutorial</b>	:	0
<b>Practical</b>	:	0

### **Course Objectives:**

[CO.1] To know and understand the reagents which are used in organic reactions and functional group transformations.

[CO.2] To know and understand the methods for C–C, C–N, and C–O single bonds formation.

[CO.3] To know and understand various models for stereochemical aspects of nucleophilic addition to carbonyl compounds.

[CO.3] To know and understand the methods for C–C, C–N, C–O multiple bonds formations.

### **Course Outcomes:**

*After completion of the course,*

[CO.1] Students will know and understand the reagents which are used in organic reactions and functional group transformations.

[CO.2] Students will know and understand the methods for C–C, C–N, and C–O bonds formation.

[CO.3] Students will know and understand various models for stereochemical aspects of nucleophilic addition to carbonyl compounds.

[CO.3] Students will know and understand methods for C–C, C–N, C–O multiple bonds formations.

## **COURSE CONTENT**

### **Unit I: Reagents in Organic Synthesis**

Use of the following reagents in organic synthesis and functional group transformations; complex metal hydrides organolithium, lithium dimethylcuprate, lithium diisopropylamide (LDA), organomagnesium (Grignard), organozinc, organocopper (Gilman & Normant) reagents in synthesis, dicyclohexylcarbodiimide, 1,3-dithiane (reactivity Umpolung), trimethylsilyl iodide, tri-*n*-butyltin hydride, Woodward and pervost hydroxylation, osmium tetroxide, DDQ, selenium dioxide, Phase transfer catalysts, crown ethers and Merrifield resin, Peterson's synthesis, Wilkinson's catalyst, Baker yeast,

### **Unit II: Single bond [C—X (X = C, O, N)] formations**

Various models (Cram, Cram chelation and Felkin-Anh models) of stereochemical aspects of nucleophilic additions to carbonyls chemistry of enolates (kinetic and thermodynamic) and enamines, enolates, lithium and boron enolates in aldol and Michael reactions, alkylation and acylation of enolates, mechanism of aldol (Mukaiyama aldol), Stobbe, Darzen, Acyloin condensations, epoxidations (Prilezhaev, Sharpless, Jacobsen and Shi), Metal catalysed C-C bond formations (Ullmann, Buchwald-Hartwig, Sonogashira, Heck, Suzuki, Stille, Nozaki-Hiyama and Kumada reactions).

### **Unit III: Multiple bond [C—X (X = C, N)] formations**

Phosphorus, nitrogen and sulfur ylids, Wittig reaction, Wittig-Honer reaction, Tebbe olefination, Julia olefination, Robinson annulation, Mannich reaction, Peterson olefination, Shapiro reaction,  $\beta$ -eliminations (Hoffman & ester pyrolysis), Cope elimination, selenoxide elimination, Cotey-Winter reaction, olefins from epoxides, olefin metathesis (Schrock's catalyst, Grubb's catalyst, ring closing metathesis, enyne metathesis, Thorpe reaction, Corey-Fuchs reaction, Ohira-Bestmann modification.

### Suggested Readings

- [1] Carey, F. A. and Sundberg, R.I., "*Advanced organic Chemistry, Part B: Reaction and Synthesis*", 5<sup>th</sup> Ed. Springer
- [2] Anslyn, E. V. and Dougherty, D. A., "*Modern Physical Organic Chemistry*", University Science Books.
- [3] Clayden, J., Greeves, N. and Warren, S., "*Organic Chemistry*", Oxford University Press.
- [4] Smith, M.B., "*Organic Synthesis*", 3s Ed., Academic Press.
- [5] Bruckner, R., "*Organic Mechanisms: Reactions, Stereochemistry and Synthesis*", Springer.



## CYE-426: Chemistry of Natural Products

(For the students of 02 Year PG Program in Chemistry)

Type	:	Elective Course
Total Credits	:	04 (Theory: 3 +Tutorial: 1)
Total Hours	:	45 Theory + 15 Tutorial
Lectures	:	03 per week
Tutorial	:	01 per week
Practical	:	0

### Course Objectives:

[CO.1] To know and understand the chemistry of natural products such as lignin, pectins, carbohydrates, terpenoids, pyrethroids and rotenoids

[CO.2] To know and understand the pathways of the oxidation of carbohydrates

[CO.3] To know and understand the biosynthesis of natural products

### Course Outcomes:

After completion of the course,

[CO.1] Student(s) will know and understand the chemistry of natural products such as lignin, pectins, carbohydrates, terpenoids, pyrethroids and rotenoids

[CO.2] Student(s) will know and understand the pathways of the oxidation of carbohydrates

[CO.3] Student(s) will know and understand the biosynthesis of natural products

### COURSE CONTENT

Natural coloring matter, general classification, method of synthesis, biosynthesis studies of carotenoids ( $\beta$ -carotene), anthocyanins (cyanine), flavones (chrysoin) and flavanol (Quercetin). Porphyrin-structure, spectral properties and synthesis, general and structure determination of Haemoglobin, chlorophyll and Bilirubin.

#### Unit I: Lignin and Pectins

Lignin: Chemical composition, structure, functions and chemistry.

Pectins: Chemical composition, structure, chemistry and commercial utilization.

#### Unit II: Carbohydrates and their Biological Oxidation

Classification of carbohydrates, reducing and non-reducing saccharides, D & L notations, Epimers, mutarotation and anomers.

Oxidation to Pyruvate: Glycolysis, Entner-Duodorf (ED) pathway, phosphoketolase pathway; aerobic pathways: Krebs citric acid cycle, electron transport. Fermentations: alcohol and lactic acid.

#### Unit III: Terpenoids

Classification, nomenclature, general methods of structure determination, chemistry and synthesis of abietic acid and gibberellic acid (gibberellin-A), farnesol, zingiberine and squalene) Biosynthetic studies on triterpenoids and tetraterpenoids.

#### Unit IV: Pyrethroids and Rotenoids

Classification, nomenclature, general methods of structure determination, chemistry and toxicity of synthetic pyrethroids and rotenoids.

#### Unit IV: Biosynthesis of Natural Products

Biosynthesis of carbohydrates (glucose), steroids (cholesterol) and alkaloids (tropane, isoquinoline, indole).

### Suggested Readings

- [1] Finar, I. L. (1956). Organic Chemistry, Volume 2: Stereochemistry and The Chemistry Natural Products, 5<sup>th</sup> Ed. Pearson Education India.
- [2] Singh, J.; Ali, S.M. & Singh, J. *Natural Product Chemistry*, Prajati Parakashan 2010.
- [3] Agarwal, O. P. *Chemistry of Organic Natural Products, Vol 1 and 2*, Goel Pub. House, 2002.
- [4] Chatwal, Gurdeep. *Chemistry of Organic Natural Products, Vol 1 and 2*, Goel Pub. House, 2002
- [5] Cooper, R., & Nicola, G. (2014). *Natural Products Chemistry: Sources, Separations and Structures*. CRC.
- [6] Schaefer, B. (2015). *Natural products in the chemical industry*. Springer.
- [7] Siddiqui A.A., Siddiqui S. *Natural Products Chemistry Practical Manual*, CBS Publishers.

## CYE-427: Organic Structure Determination

(For the students of 02 Year PG Program in Chemistry)

<b>Type</b>	:	Elective Course
<b>Total Credits</b>	:	04 (Theory: 3 +Tutorial: 1)
<b>Total Hours</b>	:	45 Theory + 15 Tutorial
<b>Lectures</b>	:	03 per week
<b>Tutorial</b>	:	01 per week
<b>Practical</b>	:	0

### Course Objectives:

[CO.1] To know and understand the fundamentals and applications of UV-Vis, infrared (IR) and 1D-NMR spectroscopic and mass spectroscopic techniques in the structure elucidation of organic compounds

[CO.2] To know and understand the principles and applications of 2D-NMR spectroscopic techniques in the structure elucidation

### Course Outcomes:

*After completion of the course,*

[CO.1] Learners will have the skills to interpret the data of UV-Vis, infrared (IR) and 1D-NMR spectroscopic and mass spectroscopic techniques.

[CO.2] Learners will know and understand the fundamentals and applications of UV-Vis, infrared (IR) and 1D-NMR spectroscopic and mass spectroscopic techniques.

[CO.3] Learners will have the skills to apply the spectroscopic techniques in the structure elucidation of organic compounds.

[CO.4] Learners will know and understand the principles and applications of 2D-NMR spectroscopic techniques in the structure elucidation.

## COURSE CONTENT

### Unit I: Electronic Spectroscopy

Electronic transitions in organic molecules, Woodward-Fieser rules for alkenes, Woodward rules for enones, aromatic compounds.

### Unit II: Infrared and Raman spectroscopy

For simple organic molecules, predicting number of active modes of vibrations, analysis of representative spectra of compounds with various functional groups, application of isotopic substitution.

### Unit III: Mass Spectrometry

Basic principles, hard and soft ionization techniques, mass analyzer in ESI-MS and MALDI MS, high resolution MS, isotope abundance, molecular ion, fragmentation processes (McL) of organic molecules, deduction of structure through mass spectral fragmentation.

### Unit IV: Nuclear Magnetic Resonance

Effect of magnetic field strength on sensitivity and resolution, chemical shift  $\delta$ , inductive and anisotropic effects on  $\delta$ , chemical structure correlations of  $\delta$ , chemical and magnetic equivalence of spins, spin-spin coupling, structural correlation to coupling constant  $J$ , first order and second order spectra, examples of AB, AX, ABX, AMX and AA'BB' systems, simplification of second order spectrum, selective decoupling, double resonance, use of chemical shift reagents for stereochemical assignments,  $^{13}\text{C}$  NMR, T1 relaxation, NOE effects, DEPT, determination of number of attached hydrogens,  $^1\text{H}$  and  $^{13}\text{C}$  chemical shifts to structure correlations, study of dynamic processes by VT NMR. restricted rotation (DMF, DMA, biphenyls, annulenes), cyclohexane ring inversion, degenerate rearrangements (fulvalene and related systems). Multinuclear NMR, COSY, DQF-COSY, HETCOR, HMQC, HMBC, TOCSY, ROESY, VGSE.

### Unit V: Spectroscopic Application

Structure elucidation of organic compounds using spectroscopic methods.

### Suggested Readings

- [1] Silverstein, R. M., Webster, F. X. and Kiemle, D., "*Spectrometric Identification of Organic Compounds*", 7th Ed., John Wiley & Sons.
- [2] Kemp, W. L., "*Organic Spectroscopy*", Palgrave.
- [3] Pavia, D. L., "*Spectroscopy*", 4<sup>th</sup> Ed., Cengage.
- [4] Williams, D. and Fleming, I., "*Spectroscopic Methods in Organic Chemistry*", 6th Ed., McGraw Hill Education (India) Private Limited.



## **CYE-428: One and Two Dimensional NMR Spectroscopic Techniques: Principals and Applications**

(For the students of 02 Year PG Program in Chemistry)

Type	:	Core Course
Total Credits	:	04 (Theory: 03 + Tutorial: 01)
Total Hours	:	45 Theory + 15 Tutorial
Lectures	:	03 per week
Tutorial	:	01 per week
Practical	:	0

### **Course Objectives:**

[CO.1] To know and understand NMR concepts, the analysis of one-dimensional NMR spectra of various nuclei, viz.,  $^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{19}\text{F}$ ,  $^{31}\text{P}$ ,  $^{119}\text{Sn}$ ,  $^{77}\text{Se}$ ,  $^6\text{Li}$ ,  $^7\text{Li}$ , etc.

[CO.2] To know and understand the spin echoes, the NOE phenomenon, and the polarization transfer mechanism,

[CO.3] To know and understand the utility of 2D NMR experiments (such as COSY, TOCSY, HSQC, HMBC, NOESY, INADEQUATE, DOSY, etc) in deriving molecular structures.

### **Course Outcomes:**

*After completing the course,*

[CO.1] Students will know and understand NMR concepts, the analysis of one-dimensional NMR spectra of various nuclei, viz.,  $^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{19}\text{F}$ ,  $^{31}\text{P}$ ,  $^{119}\text{Sn}$ ,  $^{77}\text{Se}$ ,  $^6\text{Li}$ ,  $^7\text{Li}$ , etc.

[CO.2] Students will know and understand the spin echoes, the NOE phenomenon, and the polarization transfer mechanism

[CO.3] Students will have the ability to conduct 2D NMR experiments (such as COSY, TOCSY, HSQC, HMBC, NOESY, INADEQUATE, DOSY, etc) and interpretation of the results/data/spectra for deriving the molecular structures.

### **COURSE CONTENT**

#### **Unit 1: (15 Hours)**

NMR Concepts, Spin Physics, Resonance Phenomenon, Internal interaction parameters, Chemical Shifts, factors affecting the chemical shifts, Scalar Couplings, Salient features of scalar couplings, sign of couplings, active and passive couplings, multiplicity patterns, Pople Notation

#### **Unit 2: (15 hours)**

Analysis of  $^1\text{H}$  NMR spectra, Satellite analysis,  $^{13}\text{C}$  NMR spectra, Analysis of spectra of hetero-nuclei, Spin echoes, J modulation and polarization transfer

#### **Unit 3: (15 Hours)**

2D NMR Concepts, 2D COSY, 2D COSY, TOCSY, HSQC, HMBC, INADEQUATE, J-Resolved,

#### **Unit 4: (15 Hours)**

NOE Concepts, ROESY and 2D NOESY, 1D NOESY, 1D TOCSY, Pure Shift

### **Suggested Readings:**

[1] High Resolution NMR Techniques in Organic Chemistry, Timothy D.W. Claridge

[2] NMR Data Interpretation Explained, Niel E Jacobsen

[3] NMR Spectroscopy Explained, Niel E Jacobsen

[4] Multidimensional NMR Methods for the solution state, edtrs, Gareth Morris and JW Emsley

## CYE-429: Modern Organic Synthesis Methods

(For the students of 02 Year PG Program in Chemistry)

Type	:	Elective Course
Total Credits	:	04 (Theory: 03 + Tutorial: 01)
Total Hours	:	45 Theory + 15 Tutorial
Lectures	:	03 per week
Tutorial	:	01 per week
Practical	:	0

### Course Objectives:

- [CO.1] To know and understand the various types of oxidation reactions
- [CO.2] To know and understand the modern reactions of high utility in organic synthesis
- [CO.3] To learn how to protect and deprotect the functional groups during multistep organic synthesis
- [CO.4] To know and understand the retrosynthetic approach

### Course Outcomes:

After completion of this course,

- [CO.1] Students will know and understand the various types of oxidation reactions
- [CO.2] Students will know and understand the modern reactions of high utility in organic synthesis
- [CO.3] Students will know how to protect and deprotect the functional groups during multistep organic synthesis
- [CO.4] Students will know and understand the retrosynthetic approach

## COURSE CONTENT

### Unit I: Oxidations

Oxidations of hydrocarbons (alkanes, alkenes and aromatic), alkenes to epoxides (peroxides/per acids based), Sharpless asymmetric epoxidation, Jacobsen epoxidation, Shi epoxidation, alkenes to diols (Manganese, Osmium-based), Sharpless asymmetric dihydroxylation, Prevost reaction and Woodward modification, alkenes to carbonyls with bond cleavage (manganese, osmium, ruthenium and lead based-ozonolysis), alkenes to alcohols/carbonyls without bond cleavage (hydroboration-oxidation, Wacker oxidation, selenium, chromium based allylic oxidation), ketones to  $\alpha$ -hydroxy ketones,  $\alpha,\beta$ -unsaturated ketones, ester/lactones (Baeyer-Villiger), alcohols to carbonyls (chromium, manganese, aluminum, silver, ruthenium, DMSO, hypervalent iodine and TEMPO based reagents), alcohols to acids or esters, phenols (Fremy's salt, silver carbonate).

### Unit II: Named reactions

Baylis-Hillman reaction, Henry reaction, Nef reaction, Kulinkovich reaction, Ritter reaction, Sakurai reaction, Tishchenko reaction, Ugi reaction, Brook rearrangement and Tebbe olefination.

### Unit III: Protection and Deprotection of Functional Groups

Protection and deprotection of hydroxy, carboxyl, carbonyl, carboxy amino groups and carbon-carbon multiple bonds, chemo- and regioselective protection and deprotection, illustration of protection and deprotection in multi-step synthesis.

### Unit IV: Retrosynthetic analysis:

Basic principles and terminology of retrosynthesis, guidelines, synthesis of aromatic compounds, one group and two group C-X disconnections, one group C-C and two group C-C disconnections, amine and alkene synthesis, important strategies of retro synthesis, functional group transposition, important functional group interconversions, reversal of polarity (umpolung).

### Suggested Readings

- [1] Carey, F. A. and Sundberg, R. J., "Adv. Org. Chemistry, Part B: Reactions and Synthesis", 5th Ed., Springer.
- [2] Carruthers, W. and Coldham, I., "Modern Methods of Organic Synthesis", 4th Ed., Oxford University Press.
- [3] Smith, M.B., "Organic Synthesis", 3rd Ed., Academic Press.
- [4] Stuart "Organic Synthesis"

## CYE-430: Total Organic Synthesis

(For the students of 02 Year PG Program in Chemistry)

Type	:	Elective Course
Total Credits	:	04 (Theory: 03 + Tutorial: 01)
Total Hours	:	45 Theory + 15 Tutorial
Lectures	:	03 per week
Tutorial	:	01 per week
Practical	:	0

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### Course Objectives:

- [CO.1] To know and understand the strategies for synthesis of complex molecular architectures
- [CO.2] To know and understand the total synthesis of antibiotics, alkaloids, and terpenoids.
- [CO.3] To know and understand the total synthesis of steroids and hormones.

### Course Outcomes:

After completion of this course,

- [CO.1] Students understand the strategies for synthesis of complex molecular architectures.
- [CO.2] Students will know and understand the total synthesis of antibiotics, alkaloids, and terpenoids.
- [CO.3] Students will know and understand the total synthesis of steroids and hormones.

### COURSE CONTENT

- [1] Introduction to strategies for synthesis of complex molecular architectures.
- [2] Synthesis of antibiotics - penicillin V and tetracycline.
- [3] Synthesis of alkaloids - reserpine and camptothecin.
- [4] Synthesis of terpenoids -  $\beta$ -pinene, camphor, abietic acid and  $\beta$ -amirine.
- [5] Synthesis of steroids and hormones - cholesterol, progesterone and cortisone
- [6] Synthesis of prostaglandins PGE<sub>2</sub> and PGF<sub>2</sub> $\alpha$ ; glycosidic pigments anthocyanins and quercetin; macrocyclic lactam fluvirucin-B1-aglycone; and vitamin biotin.

### Suggested Readings

- [1] Finar, I.L., "Organic Chemistry", Vol .2, 5th Ed., ELBS
- [2] Corey, E.J. and Cheng, X.-M., "The Logic of Chemical Synthesis", Wiley-VCH, Weinheim
- [2] Nicolaou, K.C. and Sorensen, E.J., "Classics in Total Synthesis", Wiley-VCH, Weinheim
- [4] Gewert, J.A., Gortlitz, J., Gotze, S., Looft, J, Menningen, P., Nobel, T., Schimek, H. and Wulff, C., "Organic synthesis workbook", Wiley-VCH, Weinheim.

## CYE-473: Named Organic Reactions Lab

(For the students of 02 Year PG Program in Chemistry)

Type	:	Elective Course
Total Credits	:	04 (Theory: 00 + Practical: 60)
Total Hours	:	60 Practicals
Lectures	:	0
Tutorial	:	0
Practical	:	04 per week

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### Course Objectives:

[CO.1] To introduce students to important carbon-carbon bond forming reactions such as Suzuki, Heck, Diels-Alder, Aldol, and Knoevenagel reactions used in organic synthesis.

[CO.2] To develop practical understanding of transition metal-catalyzed reactions and their applications in modern organic chemistry.

[CO.3] To provide hands-on experience in the synthesis, purification, and characterization of organic compounds using standard laboratory techniques.

[CO.4] To know students with the mechanism and synthetic significance of important name reactions such as Sandmeyer, Friedel-Crafts, Wittig, Cannizzaro, and Fischer indole synthesis.

### Course Outcomes:

*After completion of the course,*

[CO.1] Students will be able to perform and understand various organic synthesis reactions, including carbon-carbon bond forming and substitution reactions.

[CO.2] Students will gain the ability to apply transition metal catalysis in reactions such as Suzuki and Heck coupling.

[CO.3] Students will be able to synthesize, purify, and isolate organic compounds using techniques such as recrystallization and other purification methods.

[CO.4] Students will understand the reaction mechanisms and synthetic applications of important organic name reactions and interpret the results of laboratory experiments.

### COURSE CONTENT

[1] Suzuki reaction between organoboron reagent and haloarene in presence of transition metal catalyst

[2] Heck reaction between alkene and haloarene in presence of transition metal catalyst

[3] Diels-Alder reaction between anthracene and maleic anhydride.

[4] Aldol condensation (benzaldehyde + acetone or cinnamaldehyde + acetone)

[5] Sandmeyer reaction for Synthesis of 2-iodobenzoic acid

[6] Knoevenagel condensation between aldehyde (4-diethylaminobenzaldehyde) and malonic acid, cyanoacetic acid or malononitrile.

[7] Friedel-Crafts reaction: synthesis of 1,4-di-tert-butyl-2,5-dimethoxy benzene.

[8] Preparation and purification of cis- and trans-stilbenes by Wittig reaction.

[9] Cannizzaro reaction of an aromatic Aldehyde (p-nitrobenzaldehyde).

[10] Fisher indole synthesis.

*Note: Minimum eight experiments must be done and some would require more two-three turns.*

### Suggested Readings

[1] Arthur, I. V. Quantitative Organic Analysis, Pearson.

- [2] Furniss B.S., Handford A.J., Smith P.W.G. and Tatchell A.R., "Vogel's Text Book of Practical Organic Chemistry", 5th Ed., Longman.
- [3] Leonard J., Lygo B. and Procter G., "Advanced Practical Organic Chemistry", Chapman & Hall.
- [4] Mann, F.G. & Saunders, B.C. Practical Organic Chemistry, Pearson Education.
- [5] Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. Practical Organic Chemistry, 5th Ed., Pearson



## CYE-474: Molecular Organic Synthesis Lab

(For the students of 02 Year PG Program in Chemistry)

<b>Type</b>	:	Elective Course
<b>Total Credits</b>	:	04 (Theory: 00 + Practical: 60)
<b>Total Hours</b>	:	60 Practical's
<b>Lectures</b>	:	0
<b>Tutorial</b>	:	0
<b>Practical</b>	:	04 per week

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### Course Objectives:

[CO.1] To provide practical knowledge of functional group transformations involving carbonyl, amino, and active methylene compounds through the synthesis of their derivatives.

[CO.2] To develop understanding of important organic reactions such as oxidation, reduction, bromination, and condensation reactions used in organic synthesis.

[CO.3] To develop experimental skills in the synthesis, purification, and characterization of organic compounds and understand reaction mechanisms involved in laboratory preparations.

### Course Outcomes:

*After completion of the course,*

[CO.1] Students will be able to perform synthesis of organic derivatives of carbonyl, amino, and active methylene compounds and understand their identification.

[CO.2] Students will gain the ability to carry out oxidation, reduction, bromination, and condensation reactions for the preparation of various organic compounds.

[CO.3] Students will be able to prepare and utilize important reagents such as pyridinium dichromate and apply them in organic transformations.

## COURSE CONTENT

[1] Synthesis of derivatives for carbonyl, amino and active methylene compounds.

[2] Oxidation of hydroquinone to p-benzoquinone.

[3] Oxidation of benzoin to benzyl.

[4] Conversion of benzyl to quinoxaline.

[5] Reduction of Camphor.

[6] Synthesis of binaphthol by green reaction.

[7] Bromination of acetanilide.

[8] Preparation of p-nitroaniline of acetanilide

[9] Preparation of pyridium dichromate and its uses in oxidation of benzyl alcohol.

[10] Synthesis of  $\omega$ -nitrostyrene from an aromatic aldehyde and nitromethane

[11] Synthesis of chalcone from an aromatic aldehyde and acetophenone.

[12] Synthesis of  $\alpha$ -bromo cinnamic acid or phenyl acetylene from benzaldehyde, (formation of cinnamic acid, bromination and elimination reactions).

[13] Preparation of meso-stilbene dibromide and its conversion to diphenylacetylene.

*Note: Minimum eight experiments must be done and some would require more two-three turns.*

### Suggested Readings

[1] Arthur, I. V. Quantitative Organic Analysis, Pearson.

[2] Furniss B.S., Handford A.J., Smith P.W.G. and Tatchell A.R., "Vogel's Text Book of Practical Organic Chemistry", 5th Ed., Longman.

- [3] Leonard J., Lygo B. and Procter G., "Advanced Practical Organic Chemistry", Chapman & Hall.  
[4] Mann, F.G. & Saunders, B.C. Practical Organic Chemistry, Pearson Education.  
[5] Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. Practical Organic Chemistry, 5th Ed., Pearson



## CYE-475: Molecular Purification and Characterization Lab

(For the students of 02 Year PG Program in Chemistry)

<b>Type</b>	:	Elective Course
<b>Total Credits</b>	:	04 (Theory: 00 + Practical: 60)
<b>Total Hours</b>	:	60 Practical's
<b>Lectures</b>	:	0
<b>Tutorial</b>	:	0
<b>Practical</b>	:	04 per week

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### Course Objectives:

[CO.1] To develop understanding of chromatographic techniques such as TLC, PTLC, and column chromatography for the separation and purification of organic mixtures.

[CO.2] To introduce students to spectroscopic and instrumental methods such as UV-Visible spectroscopy, NMR spectroscopy, and gas chromatography for analysis and structure determination of organic compounds.

[CO.3] To develop experimental skills in organic synthesis, purification, and characterization of organic molecules through different laboratory reactions.

### Course Outcomes:

*After completion of the course,*

[CO.1] Students will be able to separate and purify organic mixtures using chromatographic techniques such as TLC, PTLC, and column chromatography.

[CO.2] Students will gain the ability to perform quantitative estimations of organic compounds such as aspirin and glucose using suitable analytical methods.

[CO.3] Students will be able to carry out synthesis, purification, and characterization of organic compounds and analyze reaction products using instrumental techniques such as GC and spectroscopic methods.

### COURSE CONTENT

[1] Separation of organic mixtures by TLC and PTLC.

[2] Separation of binary mixture of organic compounds using column chromatography.

[3] Calculation of  $\lambda_{max}$  of organic compounds using Woodward Fieser Rules and comparing the values with that obtained in recorded spectrum

[4] Structure elucidation of organic molecules using  $^1H$  and  $^{13}C$  NMR spectra.

[5] Gas chromatographic (GC) analysis of the mixture of catalytic oxidation of organic substrate(s)

[6] To determine the quantity of aspirin in the whole of the given solution.

[7] To estimate the quantity of glucose in the whole of the given solution.

[8] Allylation of isatin via  $S_N2$  reaction and characterization of the product

[9] Luminol synthesis from 3-nitrophthalic acid, chemiluminescence demonstration and purification and characterization of the product

[10] Preparation of anthracene from phthalic anhydride, and purification and characterization of the product

[11] Esterification of p-hydroxybenzoic acid and purification & characterization of the product

[12] Nitration of p-hydroxybenzoic acid and purification & characterization of the product

[13] Synthesis of 4-cyano-2-aminophenol from 4-hydroxybenzaldehyde, and purification & characterization of the product

*Note: Minimum eight experiments must be done and some would require more two-three turns.*

### Suggested Readings

- [1] Arthur, I. V. Quantitative Organic Analysis, Pearson.
- [2] Furniss B.S., Handford A.J., Smith P.W.G. and Tatchell A.R., "Vogel's Text Book of Practical Organic Chemistry", 5,h Ed., Longman.
- [3] Leonard J., Lygo B. and Procter G., "Advanced Practical Organic Chemistry", Chapman & Hall.
- [4] Mann, F.G. & Saunders, B.C. Practical Organic Chemistry, Pearson Education.
- [5] Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. Practical Organic Chemistry, 5th Ed., Pearson



## **CYE-441: Physical Chemistry of Surfaces and Interfaces**

(For the students of 02 Year PG Program in Chemistry)

<b>Type</b>	:	Elective Course
<b>Total Credits</b>	:	04 (Theory: 03 + Tutorial: 01)
<b>Total Hours</b>	:	45 Theory + 15 Tutorial
<b>Lectures</b>	:	03 per week
<b>Tutorial</b>	:	01 per week
<b>Practical</b>	:	0

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### **Course Objectives:**

[CO.1] To know and understand understand capillarity, surface free energy and thermodynamics of surfaces and interfaces

[CO.2] To know and understand the electrical phenomenon occurring at the interfaces

[CO.3] To know and understand various ways of measuring surface and interfacial tension

[CO.4] To know and understand the stability of colloidal systems

[CO.5] To know and understand various factors to produce stable colloidal systems (emulsions, sols, gels, dispersions, foams, etc.)

[CO.6] To know and understand about wetting and liquid repellancy on surfaces

### **Course Outcomes:**

*After completion of the course,*

[CO.1] Student(s) will know and understand the surfactants and interfacial phenomena, and thermodynamics of surfaces and interphases.

[CO.2] Student(s) will know and understand the theories, laws, and tools used in surface chemistry and forces.

[CO.3] Student(s) will know and understand the surfactants and colloid systems and their physiochemical properties.

[CO.4] Student(s) will know and understand and will be able to design methods to produce stable colloidal systems (emulsions, sols, gels, dispersions, foams, etc.)

[CO.5] Student(s) will know and understand about foams and aerosol and their applications.

## **COURSE CONTENT**

### **Unit I: Capillarity** (7 Hours)

Surface tension, Surface free energy surface-phase thermodynamics, Gibb's adsorption isotherm, Young's equation, Young-Laplace-equation and monolayers, Measurement of surface and interfacial tension

### **Unit II: Electrical Aspects of Surface Chemistry** (8 hours)

Electrical Double Layer, Free Energy of a Diffuse Double Layer, Repulsion between Two Planar Double Layers, Zeta Potential, Electrophoresis, Electroosmosis, Streaming Potential, Sedimentation Potential, Interrelationships in Electrokinetic Phenomena: Potential, Surface Charge, and Colloidal Stability

### **Unit III: Surfaces of Solids** (7 hours)

Surface Mobility of Solids Effect of Processing on the Condition of Solid Surfaces, Factors Affecting the Surface Energies and Surface Tensions of Actual Crystals State of Subdivision Deviations from Ideality, Fractal Surfaces Dislocations, Reactions of Solid Surfaces

### **Unit IV: Solid-Liquid Interface** (8 hours)

Surfactants, Micelles, Critical micelle concentration, Emulsions, Surface activity in emulsions, Stability of emulsions, Demulsification, Surface Energies from Solubility Changes Surface Energies from Immersion, Adsorption, and Engulfment Studies

**Unit V: Wetting, Flootation and Detergency** (05 hours)

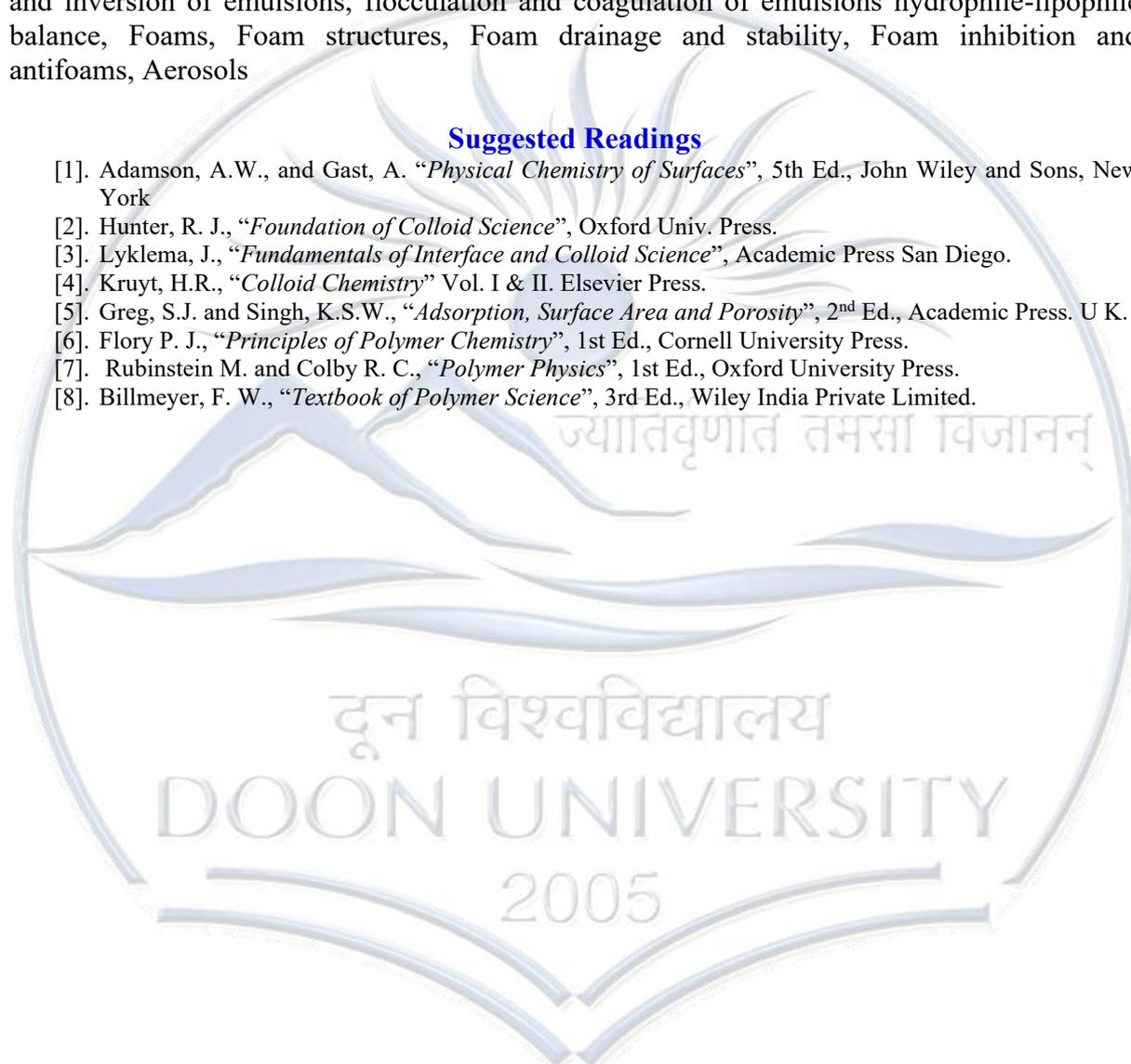
Wetting, water repellency, flootation, role of contact angle in flootation, properties of association colloids – micelles, detergency

**Unit VI: Emulsions, Foams and Aerosols** (10 hours)

Emulsions, Foams and aerosols: Emulsions, factors determining emulsion stabilization, stabilization of emulsions: long range forces, specific chemical and structural effects, ageing and inversion of emulsions, flocculation and coagulation of emulsions hydrophile-lipophile balance, Foams, Foam structures, Foam drainage and stability, Foam inhibition and antifoams, Aerosols

**Suggested Readings**

- [1]. Adamson, A.W., and Gast, A. "*Physical Chemistry of Surfaces*", 5th Ed., John Wiley and Sons, New York
- [2]. Hunter, R. J., "*Foundation of Colloid Science*", Oxford Univ. Press.
- [3]. Lyklema, J., "*Fundamentals of Interface and Colloid Science*", Academic Press San Diego.
- [4]. Kruyt, H.R., "*Colloid Chemistry*" Vol. I & II. Elsevier Press.
- [5]. Greg, S.J. and Singh, K.S.W., "*Adsorption, Surface Area and Porosity*", 2<sup>nd</sup> Ed., Academic Press. U K.
- [6]. Flory P. J., "*Principles of Polymer Chemistry*", 1st Ed., Cornell University Press.
- [7]. Rubinstein M. and Colby R. C., "*Polymer Physics*", 1st Ed., Oxford University Press.
- [8]. Billmeyer, F. W., "*Textbook of Polymer Science*", 3rd Ed., Wiley India Private Limited.



## CYE-442: Advanced Surface and Colloidal Chemistry

(For the students of 02 Year PG Program in Chemistry)

Type	:	Elective Course
Total Credits	:	04 (Theory: 4 + Practical: 0)
Total Hours	:	60 Theory + 0 Practicals
Lectures	:	04 per week
Tutorial	:	0
Practical	:	0

### Course Objectives:

[CO.1] To know and understand the surfactants and interfacial phenomena, and thermodynamics of surfaces and interphases

[CO.2] To know and understand the membranes and their applications

[CO.3] To understand the adsorption on solids/porous materials, and colloid systems and their properties

### Course Outcomes:

*After completion of the course,*

[CO.1] Student(s) will know and understand the surfactants and interfacial phenomena, and thermodynamics of surfaces and interphases.

[CO.2] Student(s) will know and understand the membranes and their applications.

[CO.3] Student(s) will know and understand the adsorption on solids/porous materials, and colloid systems and their properties.

## COURSE CONTENT

### Unit I: Surfactants and Interfacial Phenomena

Classification, micellization, c.m.c. and its determination. Shape and structure of micelles, effect of additives on micellization, thermodynamics of micellization, solubilization and applications, effect of electrolytes on solubilization. Macro and micro emulsions, dispersion and aggregation of solids by surfactants.

### Unit II: Thermodynamics of Surfaces and Interphases:

Surface and interfacial phenomenon, macromolecules, adsorption of gases by solids, BET theorem, determination of surface area of solids, adsorption from solution, electrical phenomenon of interphases. electrode- solution interface, rate of charge transfer in electrode reactions,

### Unit III: Membranes and their Applications

Artificial and natural membranes, Donnan membrane equilibrium, transport of electrolytes, membrane potential and ion selective electrodes.

### Unit IV: Adsorption on solids and porous materials

Model for multilayer adsorption, BET isotherm and application to different types of adsorbents, adsorption by porous, non-porous and microporous solids. Estimation of specific surface area and pore size distribution. Special problems encountered with very narrow pore size material and adsorption from liquid phase.

### Unit V: Colloid systems and their properties

Origin of the charges, electro-kinetic phenomena, electrophoresis, electro-osmosis, sedimentation and streaming potential. The concept of electrical double layer and various models to explain its structure and properties, DLVO theory and stability of colloids. Smoluchowski theory of kinetics of coagulation and distribution of colloids aggregates. Organic and inorganic gels and clay colloids.

### Suggested Readings

- [1] Hunter, R. J., "Foundation of Colloid Science", Oxford Univ. Press.
- [2] Lyklema, J., "Fundamentals of Interface and Colloid Science", Academic Press San Diego.
- [3] Adamson, A.W., "Physical Chemistry of Surfaces", 5th Ed., John Wiley and Sons, New York.
- [4] Kruyt, H.R., "Colloid Chemistry" Vol. I & II. Elsevier Press.
- [5] Greg, S.J. and Singh, K.S.W., "Adsorption, Surface Area and Porosity", 2<sup>nd</sup> Ed., Academic Press. U K.
- [6] Flory P. J., "Principles of Polymer Chemistry", 1st Ed., Cornell University Press.

- [7] Rubinstein M. and Colby R. C., “*Polymer Physics*”, 1st Ed., Oxford University Press.  
[8] Billmeyer, F. W., “*Textbook of Polymer Science*”, 3rd Ed., Wiley India Private Limited.



## **CYE-443: Solid State Chemistry**

(For the students of 02 Year PG Program in Chemistry)

<b>Type</b>	:	Elective Course
<b>Total Credits</b>	:	04 (Theory: 03 + Tutorial: 01)
<b>Total Hours</b>	:	45 Theory + 15 Tutorial
<b>Lectures</b>	:	03 per week
<b>Tutorial</b>	:	01 per week
<b>Practical</b>	:	0

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### **Course Objectives:**

[CO.1] To know and understand the crystal structure and symmetry in the crystalline state

[CO.2] To know and understand the applications of XRD in determine crystal structure and phase of a solid material

[CO.3] To know and understand the hard sphere model, structures derived from HCP and CCP packing, the bonding in solids, band theory, and the properties of solids

### **Course Outcomes:**

*After completion of the course,*

[CO.1] Students will know and understand the crystal structure and symmetry in the crystalline state.

[CO.2] Students will know and understand the applications of XRD in determine crystal structure and phase of a solid material.

[CO.3] Students will know and understand the hard sphere model, structures derived from HCP and CCP packing, the bonding in solids, band theory, and the properties of solids.

## **COURSE CONTENT**

### **Unit I: Symmetry in the Crystalline State:**

Crystal symmetry, elements of translation-screw axis and glide planes, symmetry in a cube, crystal classes, stereographic projection of crystal systems, space symmetry and space groups, representation of monoclinic and orthorhombic space groups.

### **Unit II: X-Ray Diffraction:**

Crystal planes and directions, Bragg's law in reciprocal space and Ewald sphere, structure factor, integrated intensity and systematic absences/presences, indexing and simulation of powder X-ray diffraction patterns for simple systems.

### **Unit III: Crystal Chemistry:**

Hard sphere model, structures derived from HCP and CCP packing, crystal structures of various compositions, derived structures and polytypes, non-stoichiometry in solids, atomic order/disorder in solids, single crystals, polycrystals, quasicrystals, amorphous / glassy solids.

### **Unit IV: Bonding in Solids:**

Bonding in molecular solids - polymorphism, bonding in extended solids ionic, covalent and metallic. Band theory of solids classification of semiconductors, metals and insulators, free electron theory, Bloch's theorem, concept of density of state and elementary band theory, band structures of one-, two- and three-dimensional solids, selected metals and insulators.

### **Unit V: Properties of solids:**

Thermal, electrical, magnetic and dielectric properties of solids.

### Suggested Readings

- [1] West, A. R., "*Solid State Chemistry and its Applications*", Reprint, Wiley India.
- [2] Rao, C.N.R. and Gopalakrishnan, J., "*New Directions in Solid State Chemistry*", 2nd Ed., Cambridge University Press.
- [3] Stout, G.H. and Jensen, L.H., "*X-Ray Structure Determination: A Practical Guide*", 2<sup>nd</sup> Ed., Wiley-Interscience.
- [4] Giacovazzo, C., Artioli, G. and Monaco, H. L., "*Fundamentals of Crystallography*", Oxford University Press.
- [5] S. Nicola, "*Magnetic Materials: Fundamentals and Device Applications*", Cambridge University Press.
- [6] Cox, P. A., "*The Electronic Structure and Chemistry of Solids*", Oxford University Press.



## **CYE-444: Advanced Quantum Chemistry**

(For the students of 02 Year PG Program in Chemistry)

<b>Type</b>	:	Elective Course
<b>Total Credits</b>	:	04 (Theory: 03 + Tutorial: 01)
<b>Total Hours</b>	:	45 Theory + 15 Tutorial
<b>Lectures</b>	:	03 per week
<b>Tutorial</b>	:	01 per week
<b>Practical</b>	:	0

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### **Course Objectives:**

[CO.1] To know and understand the approximate solutions to the Schrodinger equation

[CO.1] To know and understand the electron spin and many electrons-systems

[CO.1] To know and understand the Hartree-Fock Self-Consistent Field method

[CO.1] To know and understand molecular structures, and semiempirical molecular orbital methods I - PI electron systems

### **Course Outcomes:**

*After completion of the course,*

[CO.1] Student(s) will know and understand the approximate solutions to the Schrodinger equation

[CO.1] Student(s) will know and understand the electron spin and many electrons-systems

[CO.1] Student(s) will know and understand the Hartree-Fock Self-Consistent Field method, molecular structures, and semiempirical molecular orbital methods I - PI electron systems

## **COURSE CONTENT**

### **Unit 1: Introduction**

Vector Interpretation of Wave function, Hermitian Operator, The Generalized Uncertainty principle, The quantum Mechanical Virial Theorem, Solution of harmonic oscillator (Operator approach), Second quantization (Boson and Fermion), Quantum theory of angular momentum, One electron Atom, Spin angular momentum.

### **Unit 2: Approximate solutions to the Schrodinger Equation:**

The Variation method (Time independent and Time Dependent), Time independent perturbation theory (non – degenerate and degenerate), Time dependent perturbation theory.

### **Unit 3: Electron Spin and Many - Electron Systems**

The Antisymmetry Principle, Spin angular momenta and their Operators, The Orbital Approximation (Slater determinant, Pauli exclusion principle), Two electron wave functions.

### **Unit 4: The Hartree-Fock Self-Consistent Field Method**

The generation of Optimized orbitals, Koopman's Theorem (The Physical Significance of Orbital Energies), The electron correlation energy, Density matrix analysis of the Hartree-Fock Approximation, Natural orbitals, The matrix solution of the Hartree- Fock Equations (Roothaan's equations).

### **Unit 5: Introduction to Molecular Structure**

The Born - Oppenheimer Approximation, Solution of the Nuclear Equation, Molecular Hartree- Fock Calculations. Electronic Structure of Linear Molecule: The MO - LCAO Approximation, The Hydrogen Molecule Ion,  $H_2^+$ , The Hydrogen molecule, Molecular Configuration - Interactions, The Valence Bond Method, Molecular Perturbation Calculations. Electronic Structure of Non-linear Molecule: The  $AH_n$  molecule: Methane, Ammonia and Water, Hybrid Orbitals: The Ethylene and Benzene Molecules.

### **Unit 6: Semiempirical Molecular Orbital Methods I - PI Electron Systems**

The Huckel Approximation for Conjugated Hydrocarbons, The Pariser-Parr-Pople Method. Semiempirical Molecular Orbital Methods II - All valence – Electron systems: The Extended Huckel Method, The CNDO Method.

### Suggested Readings

- [1] Levine, I. N. “*Quantum Chemistry*”, 7th Ed., PHI Learning Pvt. Ltd., Delhi.
- [2] McQuarrie, D. A. “*Quantum Chemistry*” Reprint, Viva Books.
- [3] Atkins, P. “*Molecular Quantum Mechanics*”, 4th Ed., Oxford University Press.
- [4] Cotton, F. A., “*Chemical Applications of Group Theory*”, Reprint, Wiley Eastern
- [5] Banwell, C.N. and McCash, E.L.M., “*Fundamentals of Molecular Spectroscopy*”, 4th Ed. McGraw-Hill N. Y.
- [5] Slichter, C.P., “*Principles of Magnetic Resonance*”, Springer Verlag.
- [6] Graybeal, J.D., “*Molecular Spectroscopy*”, McGraw-Hill.



## **CYE-445: Radiation and Photochemistry**

(For the students of 02 Year PG Program in Chemistry)

<b>Type</b>	:	Elective Course
<b>Total Credits</b>	:	04 (Theory: 03 + Tutorial: 01)
<b>Total Hours</b>	:	45 Theory + 15 Tutorial
<b>Lectures</b>	:	03 per week
<b>Tutorial</b>	:	01 per week
<b>Practical</b>	:	0

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### **Course Objectives:**

To know and understand the interaction of high energy radiation with material and induced chemical changes

### **Course Outcomes:**

After completion of the course, the students will know and understand the interaction of high energy radiation with material and induced chemical changes.

## **COURSE CONTENT**

### **Unit I: Introduction**

The scope of radiation chemistry, its relation to other scientific disciplines, the interactions of directly ionising (charged particles) and indirectly ionising (neutrons, photons) radiation with a matter as starting point of radiation-chemical reaction (radiolysis).

### **Unit II: Primary Intermediate Products (PIP) of Radiolysis, their Formation and Properties:**

Excited states, cations, electrons, radicals and anions, Complex excited states: Excimers, exciplexes, plasmons. Superexcited states, Electrons generated by irradiation as the most important agents responsible for the deposition of the radiation energy in a matter, electron degradation spectrum, thermalization and solvation of electrons, Relaxation processes in excited atoms and molecules, Reactions of PIP giving the stable products of radiolysis, Track of an ionising charged particle and its structure, The types of radiation-chemical yields, ionic-pair yield M/N, its meaning and use.

### **Unit III: Stages of Radiolysis:**

Physical stage, physicochemical stage chemical stage and their products. The stage of post-effects (either chemical or biological). The kinetics of radiation-chemical processes.

### **Unit IV: Radiolysis of Gases and Liquids:**

Ionisation in noble gases, the radiolysis of selected gaseous elements, the radiolysis of N<sub>2</sub>O and its use in dosimetry, the radiolysis of water vapour, radiolysis of liquid water (including the mechanism, the properties and reactivity of radiolytic products), the influence of conditions during the irradiation on the result of radiolysis, radiolysis of the water solutions of selected inorganic compounds, the radiolysis of solutions containing Fe<sup>2+</sup> and Ce<sup>4+</sup> ions, their use in dosimetry.

### **Unit V: Photochemistry**

Quantum efficiencies of photochemical and photophysical processes, experimental techniques for continuous photolysis, Primary and secondary photochemical processes, Franck-Condon principle and its applications, rates of absorption and emission, lifetimes of electronically excited states and their fate, quenching of excited states species-dynamic and static quenching, radiationless transition and pre-dissociation, energy transfer processes.

### **Suggested Readings**

- [1] Laidler, K.J., "Reaction Kinetics", Anand Sons, New Delhi.
- [2] Amis, E.S., "Solvent Effect of Reaction Rates and Mechanism", Academic Press.
- [3] Mukherjee, K.K., "Fundamentals of Photochemistry", New Age International Pvt. Ltd., New Delhi.
- [4] Lakowicz, J.R., "Principles of Fluorescence Spectroscopy", Plenum Press, New York.
- [5] Wishart, J.F. and Nocera, D.G., "Photochemistry and Radiation Chemistry", Oxford University Press, USA.

## **CYE-446: Advanced Physical Chemistry**

(For the students of 02 Year PG Program in Chemistry)

<b>Type</b>	:	Elective Course
<b>Total Credits</b>	:	04 (Theory: 03 + Tutorial: 01)
<b>Total Hours</b>	:	45 Theory + 15 Tutorial
<b>Lectures</b>	:	03 per week
<b>Tutorial</b>	:	01 per week
<b>Practical</b>	:	0

### **Course Objectives**

1. To develop advanced understanding of chemical kinetics, including fast reactions, reaction mechanisms, and theoretical treatment of unimolecular and diffusion-controlled reactions.
2. To introduce the principles of statistical mechanics and irreversible thermodynamics and their applications to chemical processes and reaction dynamics.
3. To understand advanced quantum mechanical methods used in the description of atomic and molecular systems.
4. To familiarize students with theoretical and experimental approaches used in modern physical chemistry research.

### **Course Outcomes**

**After completion of the course, students will be able to:**

1. Analyse complex reaction mechanisms and kinetic data using theories of unimolecular reactions, linear free energy relationships, and fast reaction techniques.
2. Apply statistical mechanics and thermodynamic principles to explain molecular distributions, entropy production, and irreversible processes in chemical systems.
3. Use quantum mechanical concepts and approximation methods such as variational and perturbation techniques to solve atomic and molecular problems.
4. Interpret advanced theoretical models including Hartree-Fock and post Hartree-Fock methods for understanding electronic structure and molecular behaviour.

### **Unit I: Advanced Chemical Kinetics (20 Lectures)**

Theories of unimolecular reactions, kinetics-proton transfer and electron transfer reactions, fast reactions – rapid flow, stopped-flow and relaxation techniques, molecular beam method, diffusion controlled reactions, oscillatory reactions, linear free energy relationship, elucidation of mechanism from kinetic data.

### **Unit II : Statistical Mechanics and Irreversible Thermodynamics (25 Lectures)**

Phase space, Liouville's theorem, Maxwell-Boltzmann, Bose-Einstein, Fermi-Dirac statistics. Affinities and fluxes, reversible and irreversible processes, entropy production for some important irreversible processes, entropy flow due to exchange of matter and energy, entropy changes due to chemical reaction, affinity and coupling of chemical reaction, the phenomenological laws and equations and their applications in chemistry, fluctuations, response functions, time correlation function, distribution function.

### **Unit III: Advanced Quantum Chemistry (15 Lectures)**

Dirac Bra-ket notation, addition of angular momentum, use of ladder operators – rigid rotor and harmonic oscillator, variation method – treatment of He atom, perturbation method – examples of anharmonic oscillator, He atom, Stark and Zeeman splitting, Hartree-Fock method, introduction to post Hartree-Fock methods.

## References

1. Laidler, K. J., Reaction Kinetics, Anand Sons, New Delhi.
2. Kondepudi, D. and Prigogine, I., Modern Thermodynamics: From Heat Engines to Dissipative Structures, John Wiley & Sons.
3. Callen, H. B., Thermodynamics and an Introduction to Thermostatistics, John Wiley and Sons.
4. Bransden, B. H. and Joachain, C. J., Quantum Mechanics, Addison-Wesley.
5. Sakurai, J. J., Modern Quantum Mechanics, Pearson Education.



## **CYE-447: BioPhysical Chemistry**

(For the students of 02 Year PG Program in Chemistry)

<b>Type</b>	:	Elective Course
<b>Total Credits</b>	:	04 (Theory: 03 + Tutorial: 01)
<b>Total Hours</b>	:	45 Theory + 15 Tutorial
<b>Lectures</b>	:	03 per week
<b>Tutorial</b>	:	01 per week
<b>Practical</b>	:	0

### **Course Objectives**

1. To understand the structure and function of biological macromolecules such as proteins, enzymes, DNA and RNA in living systems.
2. To introduce the principles of bioenergetics, thermodynamics and statistical mechanics in the study of biopolymers and biochemical reactions.
3. To explain intermolecular interactions and transport processes in biological systems including membrane transport and ion conduction.
4. To familiarize students with biophysical techniques used for determining molecular properties of biopolymers.

### **Course Outcomes**

**After completion of the course, students will be able to:**

1. Describe the structure, properties and functions of major biomolecules and explain helix-coil transitions in biopolymers.
2. Apply thermodynamic and statistical concepts to understand bioenergetics, ATP hydrolysis and configuration of macromolecules.
3. Analyse intermolecular forces and binding equilibria involved in biopolymer interactions and membrane transport processes.
4. Interpret experimental methods used in biophysical chemistry such as spectroscopy, electrophoresis and hydrodynamic techniques for characterization of biopolymers.

### **COURSE CONTENT**

#### **Unit I: Biological Cell and its Constituents (10 Lectures)**

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

#### **Unit II Bioenergetics & Statistical Mechanics in Biopolymers (10 Lectures)**

Standard free energy change in biochemical reactions, exergonic, endergonic. Hydrolysis of ATP, synthesis of ATP from ADP. Chain configuration of macromolecules, statistical distribution end to end dimensions, calculation of average dimensions for various chain structures. Polypeptide and protein structures, introduction to protein folding problem.

#### **Unit III: Biopolymer Interactions (10 Lectures)**

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

#### **Unit IV: Thermodynamics and Molecular Weight of Biopolymer (15 Lectures)**

Thermodynamics of biopolymer solutions, osmotic pressure, membrane equilibrium, muscular contraction and energy generation in mechanochemical system. Evaluation of size, shape, molecular weight and extent of hydration of biopolymers by various experimental techniques. Sedimentation equilibrium, hydrodynamic methods, diffusion, sedimentation velocity, viscosity, electrophoresis and rotational motions.

#### **Unit V: Cell Membrane and Transport of Ions (8 Lectures)**

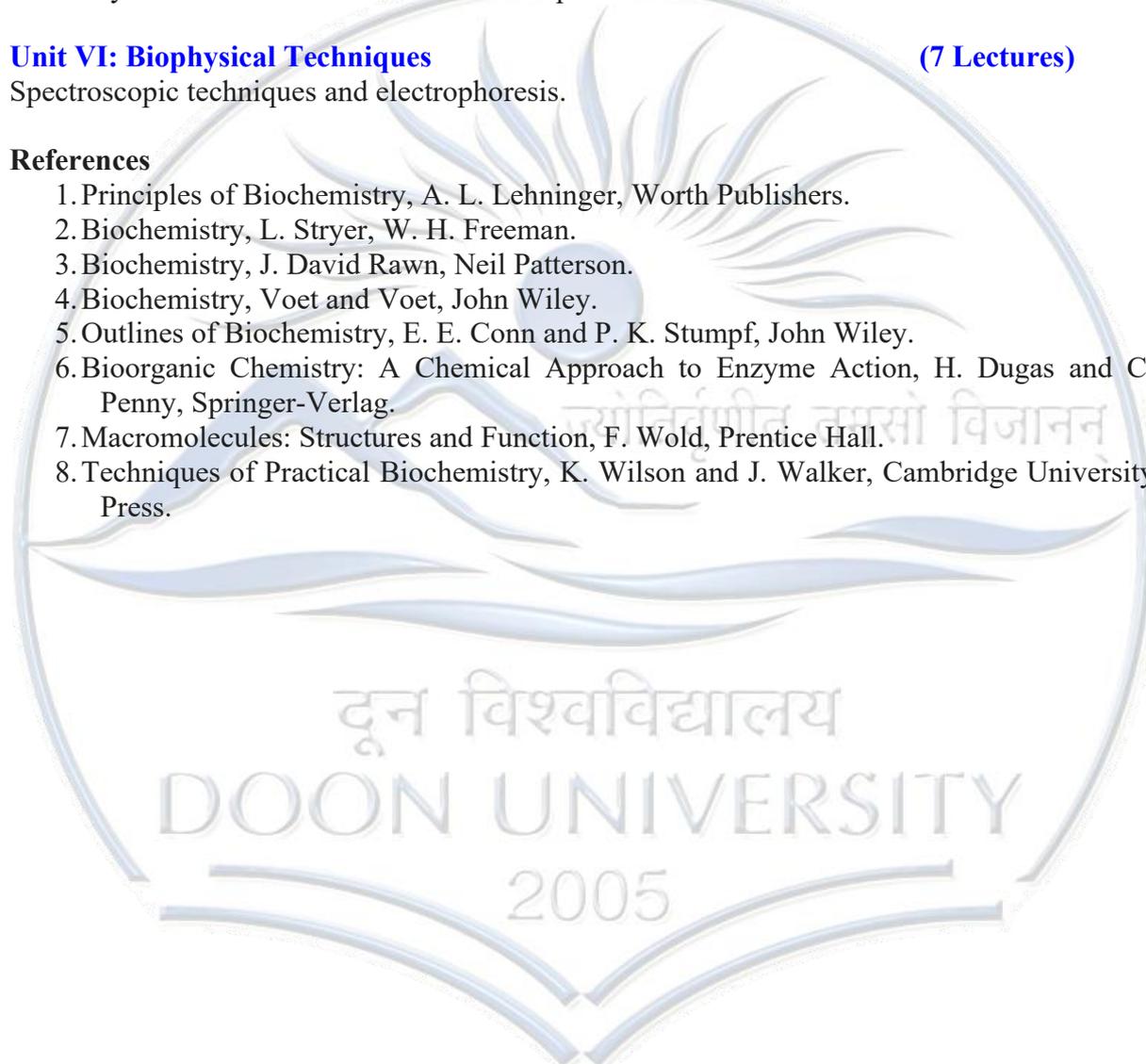
Structure and functions of cell membrane, ion transport through cell membrane, irreversible thermodynamic treatment of membrane transport. Nerve conduction.

#### **Unit VI: Biophysical Techniques (7 Lectures)**

Spectroscopic techniques and electrophoresis.

#### **References**

1. Principles of Biochemistry, A. L. Lehninger, Worth Publishers.
2. Biochemistry, L. Stryer, W. H. Freeman.
3. Biochemistry, J. David Rawn, Neil Patterson.
4. Biochemistry, Voet and Voet, John Wiley.
5. Outlines of Biochemistry, E. E. Conn and P. K. Stumpf, John Wiley.
6. Bioorganic Chemistry: A Chemical Approach to Enzyme Action, H. Dugas and C. Penny, Springer-Verlag.
7. Macromolecules: Structures and Function, F. Wold, Prentice Hall.
8. Techniques of Practical Biochemistry, K. Wilson and J. Walker, Cambridge University Press.



Discipline Specific Elective (DSE) Course in the Area of Physical Chemistry For 02 Years M.Sc. Program

## **CYE-476: Advanced Physical Chemistry Lab-I**

(For the students of 02 Year PG Program in Chemistry)

<b>Type</b>	:	Elective Course
<b>Total Credits</b>	:	04 ( Practical: 4)
<b>Total Hours</b>	:	60 Practical's
<b>Lectures</b>	:	0
<b>Tutorial</b>	:	0
<b>Practical</b>	:	04 per week

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### **Course Objectives:**

- [CO.1] To know and understand the kinetics of reactions such as, hydrolysis, saponification, of ester, decomposition, inversion of sugar dimerization
- [CO.2] To know and understand the relationship between thermodynamics parameters and how to determine these by studying kinetics of reactions and understand the concept of pK1 and pK2
- [CO.3] To know and understand the concept of equilibrium constant and Nernst distribution law
- [CO.4] To know and understand the concept of ionic strength and relation between ionic strength and reaction and rate concept of Parachor of binary mixture
- [CO.5] To know and understand the concept of surface excess concentration and thickness of interfacial adsorbed layer, surface tension
- [CO.6] To know and understand the concept critical micelle concentration and Hardy-Schultze rule for positive/negatively charged colloids
- [CO.7] To know and understand the concept of viscosity changes during a reaction
- [CO.8] To know and understand the concept of Kohlrausch's law and Ostwald's dilution law.
- [CO.9] To know and understand the concept of refractive index and molar refraction equivalent
- [CO.10] To know and understand the Beer-Lambert's law and different experimental techniques to determine composition of mixtures

### **Course Outcomes:**

*After completion of the course,*

- [CO.1] Students will know and understand the kinetics of reactions such as, hydrolysis, saponification, of ester, decomposition, inversion of sugar
- [CO.2] Students will know and understand the application of Nernst distribution law in determining equilibrium constant
- [CO.3] Students will know and understand the Beer-Lambert's law and its applications in determining concentration of a solution
- [CO.4] Students will know and understand the concept of ionic strength and relation between ionic strength and reaction rate

### **COURSE CONTENT**

- [1]. To study the kinetics of H<sup>+</sup> catalysed hydrolysis of an ester and to determine the thermodynamic parameters of the reactions
- [2]. To study the kinetics of metal catalysed decomposition of hydrogen peroxide to determine the thermodynamic parameters of the reactions

- [3]. To study the kinetics of inversion of sucrose using polarimeter
- [4]. Determination of equilibrium constant of KI<sub>3</sub> complex by distribution method.
- [5]. Verification of Beer-Lambert's law using potassium permanganate solution.
- [6]. To study the effect of ionic strength on reaction rate.
- [7]. Determination of pK<sub>1</sub> and pK<sub>2</sub> of an acid using pH meter.
- [8]. Determination of dimerization constant of benzoic acid
- [9]. Determination of surface excess concentration and thickness of interfacial adsorbed layer by surface tension measurements of water-n-butanol mixture.
- [10]. Determination of the Parachor of binary mixture of miscible solute by surface tension measurements.
- [11]. Verification of Hardy-Schultze rule for positive/negatively charged colloids.
- [12]. Determination of critical micelle concentration of sodium dodecylsulphate/cetyltrimethylammonium bromide by surface tension method.
- [13]. Determination of compound formation between liquids by viscosity variation with composition of mixtures of liquids using Ostwald viscometer.
- [14]. Determine the composition of KCl-KBr mixtures against silver nitrate solution.
- [15]. Determination of cell constant and verification of Kohlrausch's law.
- [16]. Determination of specific rotation of lactic acid/sucrose by polarimeter.
- [17]. Determination of molar refraction equivalent to -CH<sub>2</sub>, C, H, and O.
- [18]. Determination of composition of liquid mixture by refractive index measurements.
- [19]. Verification of Ostwald's dilution law

Note: Minimum eight experiments must be done and some experiments require two-three turns.

#### Suggested Readings

- [1]. Levitt, B. P., "Findlay's Practical Physical Chemistry", 9th Ed., Longman (1973).
- [2]. Garland, C.W., Nifler J.W. & Schoemaker D.P., "Experiments in Physical Chemistry" 7th Ed., McGraw-Hill International (2002).
- [3]. McGraw-Hill International (2002).
- [4]. Halpern, A. M. & Mc Bane, G. C., "Experimental Physical Chemistry", 3rd, Ed., W.H. Freeman & Co.: New York (2003).
- [6]. Experimental Physical Chemistry, F. Daniels and J. Williams.
- [7]. Advanced Physical Chemistry Experiments, Shoemaker and Gerland.

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## **CYE-477: Advanced Physical Chemistry Lab-II**

(For the students of 02 Year PG Program in Chemistry)

<b>Type</b>	:	Elective Course
<b>Total Credits</b>	:	04 ( Practical: 4)
<b>Total Hours</b>	:	60 Practical's
<b>Lectures</b>	:	0
<b>Tutorial</b>	:	0
<b>Practical</b>	:	04 per week

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### **Course Objectives:**

[CO.1] To design and execute experiments to study the kinetics of reactions under different experimental conditions.

[CO.2] To work with sol and gel systems and their viscoelastic properties.

[CO.3] To carry out electrochemical analysis for determining thermodynamic parameters.

[CO.4] To record and analyse fluorescence spectra of nanomaterials.

[CO.5] To record and analyse electronic spectra of nanomaterials and correlate it with structural properties of the same.

### **Course Outcomes:**

*After completion of the course,*

[CO.1] Students will know and understand the concept of molecular weight and molecular weight distributions in different polymers and Young's Modules of polymeric gels

[CO.2] Students will know and understand the concept and different applications of conductometric titrations

[CO.3] Students will know and understand the concept of Debye Huckle theory of ionic conductance

[Co.4] Students will know and understand the concept of fluorescence and fluorescence quenching

### **COURSE CONTENT**

[1] Determination of molecular weight of high polymer by viscometry.

[2] Determination of sparingly soluble salts solubility in water by conductometrically.

[3] To determine the equivalent conductance of weak electrolyte at infinite dilution using Kohlrausch law.

[4] Determination of Young's Modulus of soft gels.

[5] Determination of  $E_a$  of saponification of Ester by conductometry method.

[6] To determine dissociation constant of an indicator (phenolphthalein) colorimetrically.

[7] Determination of molecular radius of molecule (organic liquids) using refractometer.

[8] Determination of amount of copper by photometric titration with EDTA.

[9] Study the kinetics of iodination of acetone spectrophotometrically.

[10] Determination of glycerol radius by viscosity measurement.

[11] Verification of Debye Huckle theory of ionic conductance for strong electrolytes KCl, BaCl<sub>2</sub>, K<sub>2</sub>SO<sub>4</sub>, K<sub>3</sub>[Fe(CN)<sub>6</sub>], etc.

[12] Structural determination of metal complexes by conductometric measurement.

- [13] The partial molar volumes of sodium chloride solutions will be calculated as a function of concentration from densities measured with a pycnometer.
- [14] Kinetics of an enzyme catalyzed reaction
- [15] Kinetics of the decomposition of benzenediazonium salt.
- [16] To find the unknown concentration of a fluorophore (Quinine sulphate dehydrate) and the SternVolmer constant for fluorescence quenching

*Note: Minimum eight experiments to be performed and some experiments require two-three turns.*

### Suggested Reading

1. Experimental Physical Chemistry: A Laboratory Prescribed Book, Halpern, A. M.; McBane, G. C. 3rd ed.; W. H. Freeman, 2006.
2. Experimental Physical Chemistry, R. C. Das and Behera.
3. Advanced Practical Physical Chemistry, J. B. Yadav, Goel Publishing.
4. Experimental Physical Chemistry, F. Daniels and J. Williams.
5. Advanced Physical Chemistry Experiments, Shoemaker and Gerland.
6. Experiments in Chemistry, D. V. Jahagirdar, Himalaya Publishing House
7. Findlay's (1985): Practical Physical Chemistry, Revised and edited by B.P. Levitt 9 th edition, Longman, London



## **CYE-478: Kinetics and Photochemistry**

(For the students of 02 Year PG Program in Chemistry)

<b>Type</b>	:	Elective Course
<b>Total Credits</b>	:	04 (Theory: 03 + Tutorial: 01)
<b>Total Hours</b>	:	45 Theory + 15 Tutorial
<b>Lectures</b>	:	03 per week
<b>Tutorial</b>	:	01 per week
<b>Practical</b>	:	0

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### **Course Objectives:**

- [1] To develop a strong theoretical understanding of chemical reaction kinetics, including activation energy calculations, reaction rate theories, chain and unimolecular reactions, and the influence of reaction environment such as solvent, isotope, and catalytic effects.
- [2] To understand electron transfer processes and interfacial kinetics, encompassing homogeneous and heterogeneous systems, electron tunneling, electrode–solution interfaces, and the kinetics of electrochemical and polymerization reactions.
- [3] To provide comprehensive knowledge of photochemical and radiation-induced processes, including excited-state dynamics, quantum efficiencies, energy and charge transfer mechanisms, quenching phenomena, and a comparative understanding of photochemistry and radiation chemistry.

### **Course Outcomes:**

*After successful completion of the course, the students will be able to:*

- [CO1]: Explain and apply theoretical concepts of chemical kinetics, including activation energy calculations, reaction rate theories, and kinetics of chain, unimolecular, catalytic, and polymerization reactions.
- [CO2]: Analyze the effects of reaction conditions such as solvent, isotope substitution, salt concentration, and catalysts on reaction rates using appropriate kinetic models and experimental approaches.
- [CO3]: Interpret and evaluate electron transfer processes in homogeneous and heterogeneous systems, including electrode–solution interfaces, charge transfer rates, and kinetics of electrochemical reactions.
- [CO4]: Understand and apply principles of photochemistry and radiation chemistry, including excited-state dynamics, quantum efficiency, quenching mechanisms, energy transfer processes, and comparison of photo- and radiation-induced reactions.

## **COURSE CONTENT**

### **Unit I: Theories (10 hr)**

Theoretical calculation of energy of activation using potential energy surface diagram, absolute reaction rate theory, comparison between gas phase and solution reactions.

## **Unit II: Types of Reactions (15 hr)**

Kinetics of chain reactions, detections of radical and kinetics of HBr, elementary idea of unimolecular reactions, application of following to the reaction kinetics— solvent effect, kinetic isotope effect and salt effect, experimental technique for studying the fast reaction kinetics, kinetics of homogenous and heterogenous catalysis, kinetics of polymerization.

## **Unit III: Electron Transfer Dynamics (15 hr)**

Electron transfer in homogeneous systems, theory of electron transfer processes, electron tunneling, experimental results, electron transfer in heterogeneous systems, electrode-solution interface, rate of charge transfer in electrode reactions, study of kinetics of electrode processes.

## **Unit IV: Photochemistry (20 hr)**

Quantum efficiencies of photochemical and photophysical processes, experimental techniques for continuous photolysis, Primary and secondary photochemical processes, Franck-Condon principle and its applications, rates of absorption and emission, lifetimes of electronically excited states and their fate, quenching of excited states species-dynamic and static quenching, radiationless transition and pre-dissociation, energy transfer processes. Radiation chemistry-Interaction with matter, dosimetry, and generation of free radicals and intermediated, comparison between photo- and radiation chemistry.

### **Suggested Readings**

- [1] Laidler, K.J., “Reaction Kinetics”, Anand Sons, New Delhi.
- [2] Amis, E.S., “Solvent Effect of Reaction Rates and Mechanism”, Academic Press.
- [3] Mukherjee, K.K., “Fundamentals of Photochemistry”, New Age International Pvt. Ltd., New Delhi.
- [4] Lakowicz, J.R., “Principles of Fluorescence Spectroscopy”, Plenum Press, New York.
- [5] Wishart, J.F. and Nocera, D.G., “Photochemistry and Radiation Chemistry”, Oxford University, Press, USA.



## **CYE-461: Methods of Chemical Analysis**

(For the students of 02 Year PG Program in Chemistry)

<b>Type</b>	:	Elective Course
<b>Total Credits</b>	:	04 (Theory: 03 + Tutorial: 01)
<b>Total Hours</b>	:	45 Theory + 15 Tutorial
<b>Lectures</b>	:	03 per week
<b>Tutorial</b>	:	01 per week
<b>Practical</b>	:	0

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### **Course Objectives:**

[CO.1] To know and understand the methods which are used in chemical analysis

[CO.2] To know and understand the principles and instrumentation of electroanalytical methods (such as voltammetry and potentiometry)

[CO.3] To know and understand the principles and instrumentation of thermal methods e.g., TGA, DSC and DTA

[CO.4] To know and understand the principles and instrumentation of spectroscopic methods (such as UV-Vis Spectrophotometry, IR Spectrophotometry and AAS-AES)

### **Course Outcomes:**

After completion of the course,

[CO.1] Student(s) will have the skills to use the methods which are used in chemical analysis

[CO.2] Students will know and understand the principles and instrumentation of electroanalytical methods (such as voltammetry and potentiometry), thermal methods (e.g., TGA, DSC and DTA) and spectroscopic methods (e.g. UV-Vis Spectrophotometry, IR Spectrophotometry and AAS-AES)

## **COURSE CONTENT**

### **Unit I: Introduction:**

Brief Introduction of Qualitative Analysis and Quantitative Analysis, Outlines of Various Types of Analytical. Methods of Analysis: Classical Methods and Instrumental Methods. Properties used in various instrumental methods. Basic components of an instrument. Data domains and Types of Analytical Data Domains (Analog Domains, Digital Domains, Time Domains). Selection of An Analytical Method: Precision, Accuracy, Sensitivity, Dynamic Range, Selectivity, Efficiency.

### **Unit II: Electroanalytical Methods:**

Potentiometry & Voltammetry (dependence on technique) Overview of electroanalytical methods Comparison: Potentiometry, Voltammetry, Coulometry, Conductometry Types of electrochemical cells Electrodes: reference, indicator, auxiliary Principles of potentiometry & Voltammetry, Nernst equation and electrode potential Types of electrodes: Reference electrodes (SCE, Ag/AgCl) Indicator electrodes (glass electrode, ion-selective electrodes) Potentiometric titrations (acid-base, redox, precipitation) Instrumentation and setup Applications: pH measurement, fluoride, nitrate, and ion- selective analysis.

### **Unit III: Thermal Methods:**

Thermal Analysis Techniques, TGA, DSC and DTA , instrumentation sample holder and Furnace Microbalance, Temperature control system, Data acquisition system, Principle of DSC, Types of DSC (Heat Flux DSC vs Power Compensation DSC), Factors affecting accuracy and precision Applications of Thermal Analysis Techniques in polymers, pharmaceuticals, and metallurgy.

### **Unit IV: Spectroscopic Methods:**

Infrared spectroscopy: Interactions of light with molecules: Absorption and Scattering. Means of excitation (light sources), separation of spectrum (wavelength dispersion, time resolution), detection of the signal (heat, differential detection), interpretation of spectrum (qualitative, mixtures, resolution), Samples preparation methods and results expected. Applications and sample analysis. UV-Visible/ Near IR: Excitation sources (lasers, time resolution), wavelength dispersion (gratings, prisms, interference filters), Detection of signal (photocells, photomultipliers, diode arrays), sensitivity and Single and Double Beam instruments, Interpretation (quantification, mixtures, absorption) Atomic absorption, atomic emission, and atomic fluorescence. Excitation and getting sample into gas phase (flames, electrical discharges, plasmas), Wavelength separation and resolution (simultaneous/scanning, signal noise), Interpretation (errors due to molecular and ionic species, matrix effects, other interferences).

### **Suggested Readings**

- [1] Principles of Instrumental Analysis - 6th Edition by Douglas A. Skoog, F. James Holler, and Stanley Crouch.
- [2] Instrumental Methods of Analysis, 7th ed, Willard, Merritt, Dean, Settle.
- [3] P.W. Atkins: Physical Chemistry.
- [4] C.N. Banwell: Fundamentals of Molecular Spectroscopy.
- [5] Brian Smith: Infrared Spectral Interpretations: A Systematic Approach.



## **CYE-462: Environmental Pollutants and Analysis**

(For the students of 02 Year PG Program in Chemistry)

<b>Type</b>	:	Elective Course
<b>Total Credits</b>	:	04 (Theory: 4 + Practical: 0)
<b>Total Hours</b>	:	60 Theory + 0 Practicals
<b>Lectures</b>	:	04 per week
<b>Tutorial</b>	:	0
<b>Practical</b>	:	0

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### **Course Objectives:**

[CO.1] To know and understand the environmental chemistry of water, water pollution, water treatment options, advanced waste water treatment, analysis of major constituents/common ions/trace pollutants in water

[CO.2] To know and understand the atmosphere, atmospheric Chemistry, air pollutants, organic air pollutants, and atmospheric analysis of gases/particulates

[CO.3] To know and understand the formation, properties, and analysis of soils

[CO.4] To know and understand the toxicological chemistry, and fate of hazardous wastes.

### **Course Outcomes:**

*After completion of the course,*

[CO.1] Students will know and understand the environmental chemistry of water, water pollution, water treatment options, advanced waste water treatment, analysis of major constituents/common ions/trace pollutants in water.

[CO.2] Students will know and understand the atmosphere, atmospheric Chemistry, air pollutants, organic air pollutants, and atmospheric analysis of gases/particulates.

[CO.3] Students will know and understand the formation, properties, and analysis of soils .

[CO.4] Students will know and understand the toxicological chemistry, and fate of hazardous wastes.

## **COURSE CONTENT**

### **Unit I: Introduction**

Environmental Segments (Atmosphere, Hydrosphere, Lithosphere, Biosphere), Natural Cycles of the environment (The Hydrologic, Oxygen, Nitrogen, Phosphate and Sulphur Cycle), Commonly Used Terms

### **Unit II: Environmental Chemistry of Water**

Properties of water, The Characteristics Of Bodies Of Water, Alkalinity of water, Source and nature of acidity, Major aquatic chemical processes, Oxidation - reduction reactions in water, pE-pH diagram, Complexation, Redox Reactions Mediated By Bacteria, Nitrogen Transformation by Bacteria

### **Water Pollution**

Synthetic Organic pollutants, Soaps and Detergents, Pesticides, Polychlorinated dibenzodioxins (PCDDs) and Polychlorinated Dibenzofurans (PCDFs), Polychlorinated Biphenyls, Elemental Pollutants, Other inorganic pollutants, Eutrophication and Algal Nutrients, Acid Mine drainage, Accumulation of Salts in water, Oxygen sag curve, Regulation of water quality, Secondary standards

### **Water Treatment Operations**

Municipal water treatment for raw water, Treatment of raw water for industrial use, Waste Water Treatment, Basic processes of water treatment, Primary treatment of waste water, Secondary treatment for municipal waste water, Trickling filters, Rotating biological contactor, Activated sludge process, The significant processes that occur in biological waste treatment, Oxidation ponds.

### **Advanced Waste Water Treatment**

Removal of Suspended Solids Removal of dissolved solids, Phosphate removal (chemical treatment) Phosphate removal (biological treatment), Removal of dissolved organic compounds,

### **Analysis of Major Constituents in Water**

Water Sampling and Storage, Water Quality Measurement, Oxygen demand pH, Acidity and Alkalinity

### **Analysis of Common Ions at Low Concentrations in Water**

Ultraviolet and Visible Spectrometry, Spectrophotometric instrumentation, Analysis by direct absorption, Analysis after formation of derivative, Examples of The Use Of Other Techniques.

### **Analysis of Trace Pollutants in Water**

Bio Concentration, Accumulation in sediments, Biomagnification, Degradation, Gas liquid Chromatography (GC) Detectors, Extraction procedures or sample preparation, High Performance Liquid Chromatography (HPLC), Analysis of Metal Ions present at trace levels, Sample containers and storage, Chelation ion liquid chromatography, Speciation of Chromium by ion chromatography, Mass spectrometric detector for GC for the determination of ultratrace levels of ( $\text{ngL}^{-1}$ ) polychlorinated organic compounds

### **Unit III: The Atmosphere and Atmospheric Chemistry**

Importance of the atmosphere, Physical characteristics of the atmosphere, Major regions of the atmosphere, Evolution of the atmosphere, Earth's Radiation, Balance Carbon Dioxide In the atmosphere, Water vapour in the atmosphere, Ions and radicals in the atmosphere, Reactions involving hydroxyl and hydroperoxyl radicals, Atmospheric reactions of oxygen, Atmospheric reactions of nitrogen.

#### **Air Pollutants**

Carbon Oxides, Sources of CO pollution, Carbon Dioxide and Global Warming, Sulphur Dioxide: Sources and Removal, Nitrogen oxides in the atmosphere, Acid rain, Particles in the atmosphere.

#### **Organic Air Pollutants**

Natural source of hydrocarbons, Oxygen-containing organic compounds, Organohalide compounds, Chlorofluow carbons and depletion of ozone layer, CFC substitutes, Consequences of ozone depletion, Photo chemical smog, Chemical reactions involved in smog formation in the atmosphere, Organo nitrogen compounds, Organic particles in the atmosphere, Nitrogen oxides in the atmosphere, Acid rain, Particles in the atmosphere.

#### **Atmospheric Analysis of Gases**

Introduction Determination of time-weighted average concentrations, Determination of inorganic gaseous pollutants, Determination low-concentrations of organic pollutants, Desorption of the analyte, Determination of instantaneous concentrations, Chemiluminescence and fluorescence, Infrared spectrometry for carbon monoxide, Electrochemical sensors minimization, Gas detector tubes, Gas solid chromatography, Sampling, Gas-solid chromatographic analysis.

#### **Atmospheric Analysis of Particulates**

Measurement and Characterisation of the particulate content, Sampling methods, Determination of total organic content in the gas sample, Analysis of particulates after dissolution, Direct analysis of particulates, Drawbacks of the direct analysis.

### **Unit IV: Soil**

#### **Soil Formation and Properties**

Introduction, Kinds of Rocks and Formation of Soil, Mineral components in soil. Exchangeable cations and cation exchange capacity, Acid - Base ion exchange reaction in soils, Profile and Its Importance, Micro and macro-nutrients in soil, Nitrogen phosphorous and potassium in soil, Wastes and pollutants in soil.

#### **Analysis of Soils, Sediments and Biological Specimens**

Sampling, Sample Preparation, Extraction of the analyte and determination, Sample preparation, Plant materials, biological tissues and fluids.

### **Unit V: Toxicological Chemistry**

Toxic chemicals and toxicity, Kinetic phase and dynamic phase, Physiological responses to toxicants, Teratogenesis, mutagenesis and carcinogenesis, Toxicity of metals, inorg. compounds & org. compounds, Toxicity of some inorganic compounds

## Toxicology of Some Organic Compounds

Benzene formaldehyde & acetaldehyde, polycyclic aromatic hydrocarbons (PAHs), phenols, Nitrosamines, Isocyanates and methyl isocyanates, Organophosphates and carbates, Inhibition by carbamate insecticide, Organochlorine compounds & PCBs, Dioxins and polychlorinated biphenyls, Polychlorinated biphenyls

## Unit VI: Reactions and Fate of Hazardous Wastes

Segregation of hazardous wastes, Transport of hazardous wastes, Reactions of hazardous waste

## Hazard Waste Reduction and Minimisation and Physical Methods of Treatment of Hazardous Wastes:

Hazardous waste treatment technologies, Physical treatment methods

## Chemical Methods of Treatment of Hazardous Wastes

Chemical oxidation and reduction, Ozonolysis, Acid-base neutralization, Chemical precipitation, Hydrolysis, Ion exchange, Thermal treatment methods, Performance of hazardous wastes incinerators, Advantages of incineration, Disadvantages of incineration, Wet air oxidation, Photolysis, Biological treatment of hazardous wastes, Land treatment, Preparation of wastes for disposal.

## Suggested Readings

- [1] Aland Wild., *Soils and the environment*, Cambridge University Press, New York, 1993.
- [2] De., A.K., *Environmental Chemistry*, 4th ed., New Age international (P) Limited, New Delhi 2001.
- [3] Fifield, F.W., and P.J. Hains., *Environmental Analytical Chemistry*, 1st ed., Blackie Academic and Professional, Glasgow, UK, 1995.
- [4] Gary W. Vanloon., and Stephen J. Duffy., *Environmental chemistry, a global perspective*, Oxford university press, New York, 2000.
- [5] Gerard Kiely., *Environmental Engineering*, Irwin Mc Graw-Hill, UK, 1998.
- [6] Gilbert M. Masters., "*Introduction to Environmental Engineering and Science*" Prentice Hall of India (Private) Ltd., New Delhi, 1994.
- [7] J. Jeffrey Peirce., Ruth F. Weiner and P. Aame VesiliJld., *Environmental Pollution and control*, 4th ed., Butterworth-Heinemann, Woburn, MA, 1998.
- [8] John P. Hager., Barry J. Hansen., John F. Pusateri., William P. Imrie., and V. Ramachandran., *Extraction and Processing for the treatment and minimization of Wastes*, The Minerals, metals and Materials society., Pennsylvania, 1994.
- [9] Loconto, Paul R, *Trace environmental quantitative analysis*, Taylor and Francis, 2006.
- [10] Michael D. Lagrega., Philip L. Buckingham., and Jeffrey C. Evans., *Hazardous Waste Management*, Mc Graw-Hill, inc. New York, 1994.
- [11] Peter O' Neill., *Environmental Chemistry*, George Allen & Unwin (Publishers) Ltd, London, UK, 1985.
- [12] Pradyot Patnaik., *Handbook of Environmental Analysis*, CRC Press, Boca Raton, Florida, 1997.
- [13] Rao. C.S., *Environmental Pollution Control Engineering*, New Age International (P) Limited, New Delhi, 1991.
- [14] Roger N. Reeve., and John D. Barnes., *Environmental Analysis*, John Wiley & sons, Chichester, UK, 1994.
- [15] Stanley E. Manahan., *Environmental Chemistry*, 8th Ed., CRC Press LLC, Boca Raton, Florida, 2005.
- [16] Thomas G. Spiro., and William M. Stigliani., 2nd ed., Prentice Hall of India (P) Ltd., New Delhi, 2003.
- [17] Vladimir N. Bashkin., *Environmental Chemistry: Asian Lessons*, Kluwer Academic Publishers, Dordrecht, The Netherlands, 2003.
- [18] William F. Pickering., *Pollution Evaluation, the quantitative aspects*, Marcel Dekker, New York, 1977.

## CYE-463: Macromolecules and Nanomaterials

(For the students of 02 Year PG Program in Chemistry)

Type	:	Elective Course
Total Credits	:	04 (Theory: 4 + Practical: 0)
Total Hours	:	60 Theory + 0 Practicals
Lectures	:	03 per week
Tutorial	:	01 per week
Practical	:	0

### Course Objectives:

- [CO.1] To know and understand the surfactant aggregation
- [CO.2] To know and understand the functional polymers
- [CO.3] To know and understand the nanomaterials

### Course Outcomes:

After completion of the course,

- [CO.1] Student(s) will know and understand the surfactant aggregation, and functional polymers
- [CO.2] Student(s) will know and understand the historical perspective, effects of nanoscience and nanotechnology on various fields, and synthesis & characterization of nanoparticles.

## COURSE CONTENT

### Unit I: Surfactant Aggregation:

Micelles, Surface active agents, Classification of surface-active agents, Micellization, Hydrophobic interaction, Critical micellar concentration (cmc), Factors affecting concentration of surfactants, Counter-ion binding of micelle, Thermodynamics of micellization, Phase separation and Mass action models, Solubilization Emulsions, Mechanism of formation of microemulsion and their stability, Physical techniques, Applications.

### Unit II: Functional Polymers:

Smart materials -uses of smart materials in sensing devices and communication networks, conducting polymers: Electrically conducting polymers and their uses. Photoconductive polymers. Liquid crystal polymers - smectic, nematic and cholesteric structures. Ionic exchange polymers: Cationic and anionic exchange polymers and their uses. Eco- friendly polymers, Membrane separation. Filtration- micro, ultra and nanofiltration. Liquid separation- dialysis, electro osmosis and reverse osmosis, Fire retarding polymers, photonic polymers. Inter penetrating networks (IPN), polymers, Polymers in biomedical applications - artificial organs and controlled drug delivery.

### Unit III: Nanomaterials:

Definition, historical perspective and effects of nanoscience and nanotechnology on various fields. Synthesis of nanoparticles by chemical routes and characterization techniques: Thermodynamics and kinetics of nucleation; Growth of polyhedral particles by surface reaction, Ostwald ripening, size distribution; TEM; SEM; AFM; Light scattering; XPS. Properties of nanostructured materials: Preparation by sol-gel and hydrothermal methods, Optical properties; magnetic properties; chemical properties. Overview of applied chemistry of Nanomaterials.

### Suggested Readings

- [1] G. C. Bond, *Principles of Heterogeneous Catalysis in practice*, Oxford Publishing.
- [2] C. Satterfield, *Heterogeneous Catalysis*, McGraw Hill
- [3] *Catalysis, Principles and applications*, edited by B. Vishwanathan, S. Sivasanker & A. V.
- [4] *Textbook of Polymer Science*, F. W. Billmeyer Jr, John Wiley & sons
- [5] *Polymer Science*, V. R. Gowarikar, N. V. Viswanathan & J. Sreedhar, Wiley Eastern
- [6] *Contemporary Polymer Chemistry*, H.R. Alcock & F. W. Lambe, Prentice Hall
- [7] *Physics and Chemistry of Polymers*, J.M. G.Cowie, Blackie Academic and professional
- [8] *Introduction to polymer Chemistry*, By Charles E Carraher Jr (Taylor- Francis)
- [9] *Solid State and its Applications* by A.R. West.
- [10] *New directions in solid state chemistry*, J. Gopalakrishnan and C.N. R. Rao.



## CYE-464: Green Methods of Synthesis

(For the students of 02 Year PG Program in Chemistry)

Type	:	Elective Course
Total Credits	:	04 (Theory: 4 + Practical: 0)
Total Hours	:	60 Theory + 0 Practicals
Lectures	:	03 per week
Tutorial	:	01 per week
Practical	:	0

### Course Objectives:

- [CO.1] To know and understand the need and principles of green chemistry
- [CO.2] To know and understand the methods for green syntheses of organic compounds
- [CO.3] To know and understand the use of microwaves and ultrasound in green syntheses
- [CO.4] To know and understand the future trends in green chemistry

### Course Outcomes:

After completion of the course,

- [CO.1] Student(s) will know and understand the need and principles of green chemistry
- [CO.2] Student(s) will know and understand the methods for green syntheses of organic compounds, and the use of microwaves and ultrasound in green syntheses
- [CO.3] Student(s) will know and understand the future trends in green chemistry

## COURSE CONTENT

### Unit I: Introduction to Green Chemistry

What is Green Chemistry? Need for Green Chemistry. Goals of Green Chemistry. Limitations/Obstacles in the pursuit of the goals of Green Chemistry.

### Unit II: Principles of Green Chemistry and Designing a Chemical synthesis

Twelve principles of Green Chemistry with their explanations and examples; Designing a Green Synthesis using these principles; Prevention of Waste/ byproducts; maximum incorporation of the materials used in the process into the final products (Atom Economy); prevention/ minimization of hazardous/ toxic products; designing safer chemicals - different basic approaches to do so; selection of appropriate auxiliary substances (solvents, separation agents), green solvents, solventless processes, immobilized solvents and ionic liquids; energy requirements for reactions - use of microwaves, ultrasonic energy; selection of starting materials; avoidance of unnecessary derivatization - careful use of blocking/protecting groups; use of catalytic reagents (wherever possible) in preference to stoichiometric reagents; designing of biodegradable products; prevention of chemical accidents; strengthening/development of analytical techniques to prevent and minimize the generation of hazardous substances in chemical processes.

### Unit III: Examples of Green Synthesis/ Reactions

1. **Green Synthesis of the Compounds:** such as adipic acid, catechol, BHT, methyl methacrylate, urethane, aromatic amines (4-aminodiphenylamine), benzyl bromide, acetaldehyde, disodium iminodiacetate (alternative to Strecker synthesis), citral, ibuprofen, paracetamol, furfural.
2. **Microwave Assisted Reactions in Water:** Hofmann Elimination, Hydrolysis (of benzyl chloride, benzamide, n-phenyl benzamide, methylbenzoate to benzole acid), Oxidation (of toluene, alcohols).  
*Microwave Assisted Reactions in Organic Solvents:* Esterification, Fries rearrangement, Orthoester Claisen Rearrangement, Diels-Alder Reaction, Decarboxylation. *Microwave Assisted Solid State Reactions:* Deacetylation, Deprotection. Saponification of esters, Alkylation of reactive methylene compounds, reductions, synthesis of nitriles from aldehydes; anhydrides from dicarboxylic acid; pyrimidine and pyridine derivatives; 1,2-dihydrotriazine derivatives; benzimidazoles.

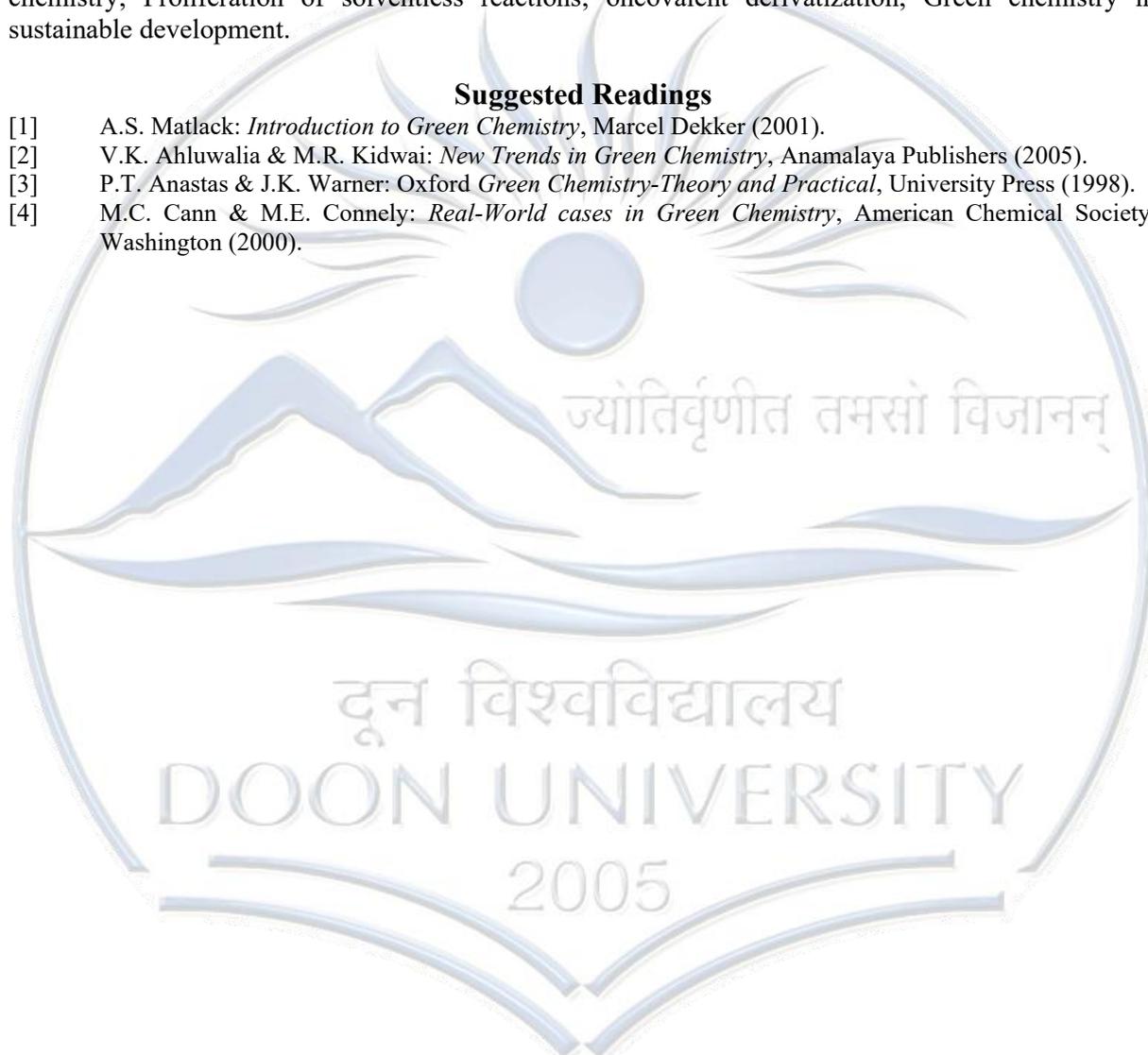
3. **Ultrasound Assisted Reactions:** Esterification, saponification, substitution reactions, Alkylations, oxidation, reduction, coupling reaction, Cannizzaro reaction, Strecker synthesis, Reformatsky reaction.
4. **Selective Methylation of Active Methylene Group using Dimethylcarbonate:** Solidstate polymerization of amorphous polymers using diphenylcarbonate; Use of "Clayan", a nonmetallic oxidative reagent for various reactions; Free Radical Bromination; Role of Tellurium in organic syntheses; Biocatalysis in organic syntheses.

#### Unit IV: Future Trends in Green chemistry

Oxidation reagents and catalysts; Biomimetic, multifunctional reagents; Combinatorial green chemistry; Proliferation of solventless reactions; oncovalent derivatization; Green chemistry in sustainable development.

#### Suggested Readings

- [1] A.S. Matlack: *Introduction to Green Chemistry*, Marcel Dekker (2001).  
[2] V.K. Ahluwalia & M.R. Kidwai: *New Trends in Green Chemistry*, Anamalaya Publishers (2005).  
[3] P.T. Anastas & J.K. Warner: *Oxford Green Chemistry-Theory and Practical*, University Press (1998).  
[4] M.C. Cann & M.E. Connely: *Real-World cases in Green Chemistry*, American Chemical Society, Washington (2000).



## CYS-403: Laboratory Skills for Physical Chemistry

(Skill Enhancement Course: 02 Credits and 60 Contact Hours)

<b>Type</b>	:	Skil Enhancement Course
<b>Total Credits</b>	:	02 (Practical: 02)
<b>Total Hours</b>	:	60 Practicals
<b>Lectures</b>	:	0
<b>Tutorial</b>	:	0
<b>Practical</b>	:	02 per week

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### Course Objectives:

- [CO.1] To know and understand the concept of miscibility
- [CO.2] To know and understand the concept of critical solution temperature and effect of impurities on CST and miscibility
- [CO.3] To know and understand the relationship between cell potential and thermodynamic parameters
- [CO.4] To know and understand the process of adsorption theories related to this phenomenon
- [CO.5] To know and understand the kinetics of hydrolysis reaction
- [CO.6] To know and understand the magnetic nature of the solids
- [CO.7] To know and understand the concept of surface plasmon resonance

### Course Outcomes:

*After completion of the course,*

- [CO.1] Students will know and understand the concept of miscibility and CST and how to measure it quantitatively
- [CO.2] Students will know and understand effect of impurities on the solubility and CST of different components and how to quantify it experimentally
- [CO.3] Students will know and understand the applications of Langmuir and Freundlich adsorption isotherm to calculate adsorption capacity and also to understand nature of adsorption
- [CO.4] Students will know and understand the kinetics of hydrolysis reaction and how to use polarimeter to determine rate of hydrolysis
- [CO.5] Students will know and understand the concept magnetic susceptibility of solids and how to measure it experimentally.
- [CO.6] Students will know and understand the concept of surface plasmon resonance in different systems and their determination using spectrophotometry

### COURSE CONTENT

- [1] To study the variation in miscibility of phenol in water with temperature and to find out the critical solution temperature (CST) and also to investigate the effect of impurities on CST.
- [2] To determine the cell potentials for different electrochemical cells and also to measure different thermodynamic parameters.
- [3] Verification of Freundlich's adsorption isotherms and calculation of characteristic constants.
- [4] Verification of Langmuir adsorption isotherms and determination of surface area.
- [5] Rate of Hydrolysis of Sucrose using polarimeter.
- [6] Determination of isotherm for three component system.

[7] To determine the magnetic susceptibility of solids.

[8] To determine refractive index of dielectric layer using SPR

*Note: Minimum five experiments must be done and some would require more two-three turns.*

### **Suggested Readings**

[1] Levitt, B.P., "*Findlay's Practical Physical Chemistry*", 9th Ed., Longman Garland C.W.,

[2] Nifler J.W. and Schoemaber D.P., "*Experiments in Physical Chemistry*", 7th Ed., JMCGra,-Hill International.

[3] Halpem, A. M. & McBane, G. C., "*Experimental Physical Chemistry 3<sup>rd</sup> Ed.*"; W.H. Freeman & Co.: New York



## CYS-404: Experimental Skills for Physical Chemistry

(Skill Enhancement Course: 02 Credits and 60 Contact Hours)

<b>Type</b>	:	Skil Enhancement Course
<b>Total Credits</b>	:	02 ( Practical: 02)
<b>Total Hours</b>	:	60 Practicals
<b>Lectures</b>	:	0
<b>Tutorial</b>	:	0
<b>Practical</b>	:	02 per week

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### Course Objectives:

[CO.1] To know and understand the kinetics of reactions such as, hydrolysis, saponification, of ester, decomposition, inversion of sugar. dimerization

[CO.2] To know and understand the relationship between thermodynamics parameters and how to determine these by studying kinetics of reactions

[CO.3] To know and understand the concept of equilibrium constant and Nernst distribution law

[CO.4] To know and understand the Beer-Lambert's law

[CO.5] To know and understand the concept of ionic strength and relation between ionic strength and reaction rate

[CO.6] To know and understand the concept of  $pK_1$  and  $pK_2$

### Course Outcomes:

*After completion of the course,*

[CO.1] Students will know and understand the the kinetics of reactions such as, hydrolysis, saponification, of ester, decomposition, inversion of sugar

[CO.2] Students will know and understand the relationship between thermodynamics parameters and how to determine these by studying kinetics of reactions

[CO.3] Students will know and understand the application of Nernst distribution law in determining equilibrium constant

[CO.4] Students will know and understand the understand the Beer-Lambert's law and its applications in determining concentration of a solution

[CO.5] Students will know and understand the concept of ionic strength and relation between ionic strength and reaction rate

[CO.6] Students will know and understand the concept of  $pK_1$  and  $pK_2$  and how to determine it using pH meter

### COURSE CONTENT

[1] To study the kinetics of  $H^+$  catalysed hydrolysis of an ester and to determine the thermodynamic parameters of the reactions

[2] To study the kinetics of saponification of ester to determine the thermodynamic parameters of the reactions

[3] To study the kinetics of metal catalysed decomposition of hydrogen peroxide to determine the thermodynamic parameters of the reactions

- [4] To study the kinetics of inversion of sucrose using polarimeter
- [5] Determination of equilibrium constant of  $KI_3$  complex by distribution method.
- [6] Verification of Beer-Lambert's law using potassium permanganate solution.
- [7] To study the quenching of fluorescence and organic dye(s).
- [8] To study the effect of ionic strength on reaction rate.
- [9] Determination of  $pK_1$  and  $pK_2$  of an acid using pH meter.
- [10] Determination of dimerization constant of benzoic acid

*Note: Some experiments require two-three turns.*

#### **Suggested Readings**

- [1] Levitt, B. P., "*Findlay's Practical Physical Chemistry*", 9<sup>th</sup> Ed., Longman (1973).
- [2] Garland, C.W., Nifler J.W. & Schoemaber D.P., "*Experiments in Physical Chemistry*". 7<sup>th</sup> Ed., McGraw-Hill International (2002).
- [3] Halpern, A. M. & Mc Bane, G. C., "*Experimental Physical Chemistry*", 3<sup>rd</sup>, Ed., W.H. Freeman & Co.: New York (2003).



## CYS-405: Physical Chemistry Lab-III

(Skill Enhancement Course: 02 Credits and 60 Contact Hours)

<b>Type</b>	:	Skill Enhancement Course
<b>Total Credits</b>	:	02 ( Practical: 02)
<b>Total Hours</b>	:	60 Practicals
<b>Lectures</b>	:	0
<b>Tutorial</b>	:	0
<b>Practical</b>	:	02 per week

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### Course Objectives:

- [CO.1] To know and understand the concept of surface excess concentration and thickness of interfacial adsorbed layer, surface tension
- [CO.2] To know and understand the concept of Parachor of binary mixture
- [CO.3] To know and understand the concept of Hardy-Schultze rule for positive/negatively charged colloids
- [CO.4] To know and understand the concept of critical micelle concentration
- [CO.5] To know and understand the concept of viscosity changes during a reaction
- [CO.6] To know and understand the concept of Kohlrausch's law and Ostwald's dilution law.
- [CO.7] To know and understand the concept of refractive index and molar refraction equivalent
- [CO.8] To know and understand the different experimental techniques to determine composition of mixtures

### Course Outcomes:

*After completion of the course,*

- [CO.1] Students will know and understand the concept of concept of surface excess concentration and thickness of interfacial adsorbed layer, surface tension and how to experimentally measure it
- [CO.2] Students will know and concept of Parachor and how to determine it experimentally for a binary mixture
- [CO.3] Students will know and understand the concept of critical micelle concentration and how to determine it by doing surface tension measurements
- [CO.4] Students will know and understand the Hardy-Schultze rule for positive/negatively charged colloids
- [CO.5] Students will know and understand the concept of viscosity changes during reaction and how it can be used to determine compound formation between liquids using Ostwald viscometer
- [CO.6] Students will know and understand the concept of Kohlrausch's law and Ostwald's dilution law
- [CO.7] Students wknow and understand the concept of refractive index and molar refraction equivalent and how to determine the composition of liquid mixtures using refractive index measurement

### COURSE CONTENT

- [1] Determination of surface excess concentration and thickness of interfacial adsorbed layer by surface tension measurements of water-n-butanol mixture.

- [2] Determination of the Parachor of binary mixture of miscible solute by surface tension measurements.
- [3] Verification of Hardy-Schultze rule for positive/negatively charged colloids.
- [4] Determination of critical micelle concentration of sodium dodecylsulphate/cetyltrimethylammonium bromide by surface tension method.
- [5] Determination of compound formation between liquids by viscosity variation with composition of mixtures of liquids using Ostwald viscometer.
- [6] Determine the composition of KCl-KBr mixtures against silver nitrate solution.
- [7] Determination of cell constant and verification of Kohlrausch's law.
- [8] Determination of specific rotation of lactic acid/sucrose by polarimeter.
- [9] Determination of molar refraction equivalent to  $-\text{CH}_2$ , C, H, and O.
- [10] Determination of composition of liquid mixture by refractive index measurements.
- [11] Verification of Ostwald's dilution law.

Note: Minimum five experiments must be done and some require two-three turns.

### Suggested Readings

- [1] Levitt, B.P., "Findlay's Practical Physical Chemistry", Ed., Longman (1973).
- [2] Garland C.W., Nifler J.W. and Schoemaber D.P., "*Experiments in Physical Chemistry*", 7<sup>th</sup> Ed., McGraw-Hill International (2002).
- [3] Ewing G.W., "Instrumental Methods of Chemical Analysis", 5th Ed., McGraw Hill (2004).
- [4] Halpern, A. M. & McBane, G. C. Experimental Physical Chemistry 3rd Ed: W.H. Freeman & Co.: New York (2003).

