# RANI RASHMONI GREEN UNIVERSITY TARAKESWAR, HOOGHLY



CBCS Syllabus
of
Master of Science (M.Sc)
in
Chemistry

Under Semester System
Course Duration: 2 years, 4 Semesters
[W.e.f.: 2025-2026]

## **Subject Chemistry**

## Programme structure

Semester	Course Code	Course Title	Full	Credit	Lecture
	EVC	E :	Marks	(L+T+P)	hours
Ι	EVS	Environmental Science	40+ <b>10*</b>	4 (4-0-0)	70
	CEM-101	Inorganic Chemistry General I	40+10	4 (4-0-0)	70
	CEM -102	Organic Chemistry General I	40+10	4 (4-0-0)	70
	CEM -103	Physical Chemistry General I	40+10	4 (4-0-0)	70
	CEM -194	Inorganic Chemistry Practical I	40+10	4 (1-1-4)	90
	CEM -195	Organic Chemistry Practical I	40+10	4 (1-1-4)	90
	Total		300	24	390
	CEM -201	CBCS-I ( Fundamentals of food and drugs)	40+10	4 (4-0-0)	70
	CEM -202	Inorganic Chemistry General II	40+10	4 (4-0-0)	70
	CEM -203	Organic Chemistry General II	40+10	4 (4-0-0)	70
II	CEM -204	Physical Chemistry General II	40+10	4 (4-0-0)	70
	CEM -295	Inorganic Chemistry Practical II	40+10	4 (1-1-4)	90
	CEM -296	Physical Chemistry Practical I	40+10	4 (1-1-4)	90
	Total		300	24	390
	CEM -301	CBCS-II (Building	40+10	4 (4-0-0)	70
		Materials, Medicinal Plants and Polymers)			
	CEM -302	Inorganic Chemistry General III	40+10	4 (4-0-0)	70
Ш	CEM -303	Organic Chemistry General III	40+10	4 (4-0-0)	70
	CEM -304	Physical Chemistry General III	40+10	4 (4-0-0)	70
	CEM -395	Physical Chemistry Practical II	40+10	4 (1-1-4)	90
	CEM -396	Organic Chemistry Practical II	40+10	4 (1-1-4)	90
	Total		300	24	390
	CEM -401	Advanced General I	40+10	4 (4-0-0)	70
	CEM -402I/ 402O/ 402P	Inorganic Chemistry Special - I/ Organic Chemistry Special - I/ Physical Chemistry Special - I	40+10	4 (4-0-0)	70
IV	CEM -403I/ 403O/ 403P	Inorganic Chemistry Special - II/ Organic Chemistry - II/ Physical Chemistry - II	40+10	4 (4-0-0)	70
	CEM -404	Grand Viva	40+10	4 (0-4-0)	70
	CEM – 495	Project	50	4 (1-1-4)	90
	CEM - 496	Internship	50	4 (1-1-4)	90
	Total	<u>I</u>	300	24	460
Grand T	<u> </u>		1200	96	<del>                                     </del>

Theory -50 Marks, Written - 40 Marks, Internal Assessment -10 Marks Theory - Marks, Written -.... Marks, Internal Assessment -... Marks Practical -100 Marks

<sup>\*</sup>Each student will obtain marks based on the plantation and growing up of a sapling that would produce fruits and attract the birds/animals.

## **Overview**

Semester	Paper	No of Papers	Full Marks of Each Paper	Total Marks Of Theoretical/ Practical Paper	Total Marks	Credit Points	Total Credit Point
1st	Theoretical	4	40+10=50	200	300	16	24
	Practical	2	50	100		8	
2nd	Theoretical	4	40+10=50	200	300	16	24
	Practical	2	50	100		8	
3rd	Theoretical	4	40+10=50	200	300	16	24
	Practical	2	50	100		8	
<b>4</b> th	Theoretical	4	40+10=50	200	300	16	24
	Project Intership	1 1	50 50	100		4	

**Grand Total= 96 Credit Points** 

## **Program outcome (P.O):**

The postgraduate program in Chemistry at Rani Rashmoni Green University aims to provide a platform for students to accrue comprehensive understanding of the major fields of chemistry. This program will prepare them for careers in research and development, while also fostering their professional growth. Additionally, the program emphasizes the development of ethical and moral values, equipping students to understand and address issues related to the environment and sustainability. Clear and compelling outcomes of the program are outlined below.

## i. Core Knowledge

Develop a strong foundation by accruing in depth knowledge of Analytical, Inorganic, Organic and Physical Chemistry together with fundamentals of Computational and Theoretical Chemistry.

## ii. Analyzing skill

Gain practical skills to prepare and analyze chemicals and materials of immediate need and to understand physicochemical principles relevant to chemical and allied industries.

## iii. Effective communication

Empower students with effective communication skills for collaborative research work on current issues, public outreach of scientific technologies, and for their career advancement.

## iv. Reflective thinking, scientific reasoning and team work.

Apply their knowledge and skills to foster their own intellectual growth. This includes developing evidence-based thinking and mastering the scientific method. Graduates will be able to seek logical explanations for the phenomena around them, whether working independently or as part of a team

## v. Moral and ethical awareness for society and environment:

Understand and apply principles of green chemistry to minimize environmental impact and waste, and to uphold professional integrity, prioritize safety, engage in responsible conduct, commit to social and environmental responsibility, and make ethical decisions.

## vi. Multicultural competency and Self-directed lifelong learning:

These skills are vital for success in a globalized world and for navigating a constantly evolving scientific landscape. Adopted methods of teaching learning process in RRGU that include problem-based theoretical and experiential learning, use of digital resources for literature survey, participation in seminars/conferences, conducting internship, and industrial visit, will significantly enhance such skills of students.

Paper	Course	Marks	Lecture	Credit Point
			hours	Creater office
CEM-101	Inorganic Chemistry I	40+10	70	4
Unit I	Selected Topics on the Chemistry of s- and p-Block Elements			
Unit II	Coordination Chemistry I			
Unit III	Environmental Chemistry			
Unit IV	Nuclear Chemistry			
Unit V	Organometallic Chemistry I			
CEM -102	Organic Chemistry General I	40+10	70	4
Unit I	Electronic property of conjugated organic systems			
Unit II	Stereochemistry 1			
Unit III	Pericyclic reactions			
Unit IV	NMR spectroscopy & Mass spectrometry			
Unit V	Natural product 1			
CEM -103	Physical Chemistry General I	40+10	70	4
Unit I	Quantum Chemistry-1			
Unit II	Symmetry and Group theory-1			
Unit III	Spectroscopy-1			
Unit IV	Atomic Structure			
Unit V	Photochemistry-1			
CEM -104	Inorganic Chemistry Practical I	50	90	4
CEM -105	Organic Chemistry Practical I	50	90	4
	Total Marks	300		
	Total Credit			24

	2 <sup>nd</sup> Semester			
Paper	Course	Marks	Lecture hours	Credit Point
CEM -201	CBCS-I ( Fundamentals of food and drugs)	40+10	70	4
Unit I	Constituents of Food			
Unit II	Introduction to food microbiology			
Unit III	Food preservation			
Unit IV	Basic principle of Pharmacology			
CEM-202	Inorganic Chemistry II	40+10	70	4
Unit I	Selected Topics on the Chemistry of d- Block Elements			
Unit II	Coordination Chemistry II			
Unit III	Complexes in Aqueous Solutions			
Unit IV	Chemical bonding			
Unit V	Errors in Chemical Analyses			
CEM-203	Organic Chemistry General II	40+10	70	4
Unit I	Reagents and rearrangement reactions			
Unit II	Heterocyclic chemistry-1			
Unit III	Logic in organic synthesis			
Unit IV	Organo-boron,-phosphorus and -sulfur, Basics of transition metal based organometallics			
Unit V	Photochemistry			
<b>CEM-204</b>	Physical Chemistry General II	40+10	70	4
Unit I	Quantum Chemistry-2			
Unit II	Symmetry and Group theory-2			
Unit III	Chemical Kinetics-1			
Unit IV	Chemical Thermodynamics-1			
Unit V	Solid state Chemistry			
CEM-295	Inorganic Chemistry Practical II	50	90	4
<b>CEM-296</b>	Physical Chemistry Practical I	50	90	4
	Total Marks	300		
	Total Credit			24

	3 <sup>rd</sup> Semester: Spl.			
Paper	Course	Marks	Lecture hours	Credit Point
<b>CEM 301</b>	CBCS-II (Building Materials, Medicinal Plants	40+10	70	4
Unit I	and Polymers) Building materials			
Unit II	Common Medicinal Plants and Their Active			
Omt n	Constituents			
Unit III	Introduction to Polymer chemistry			
Unit IV	Natural and semi-synthetic Carbohydrate Polymers			
<b>CEM 302</b>	Inorganic Chemistry general III	40+10	70	4
Unit I	Selected Topics on the Chemistry of f- Block Elements and Superheavy Elements			
Unit II	Bioinorganic Chemistry-I			
Unit III	Organometallic Chemistry II			
Unit IV	Physical Characterization of Inorganic Compounds – I			
Unit V	Inorganic Reaction Mechanism			
<b>CEM 303</b>	Organic Chemistry General III	40+10	70	4
Unit I	Stereochemistry-2			
Unit II	Linear Free Energy Relationship			
Unit III	Name reactions			
Unit IV	Medicinal chemistry			
Unit V	Polymer chemistry			
<b>CEM 304</b>	Physical Chemistry General III	40+10	70	4
Unit I	Spectroscopy-2			
Unit II	Chemical Kinetics-2			
Unit III	Computational Chemistry			
Unit IV	Colloids and surface			
Unit V	Electrochemistry: Ions in solution			
<b>CEM 395</b>	Physical Chemistry Practical II	50	90	4
<b>CEM 396</b>	Organic Chemistry Practical II	50	90	4
	Total Marks	300		
	Total Credit			24

	4th Semester: Spl.			
Paper	Course	Marks	Lecture hours	Credit Point
<b>CEM 401</b>	Advanced General I	40+10	70	4
Unit I	Separation Techniques			
Unit II	Supramolecular Chemistry			
Unit III	Materials Chemistry			
Unit IV	Crystallography			
Unit V	Green Chemistry			
<b>CEM-402I</b>	Inorganic Chemistry Special - I	40+10	70	4
Unit I	Inorganic Chains, Cages and Clusters			
Unit II	Bioinorganic Chemistry II			
Unit III	Magnetochemistry			
Unit IV	Electrochemical Analysis			
Unit V	Physical Characterization of Inorganic Compounds-II			
CEM-402O	Organic Chemistry Special-I	40+10	70	4
Unit I	Organometallic Chemistry			
Unit II	Application of Advanced NMR and Mass Spectrometry			
Unit III	Carbohydrate Chemistry			
Unit IV	Heterocyclic Chemistry-2			
Unit V	Supramolecular chemistry			
<b>CEM-402P</b>	Physical Chemistry Special-I	40+10	70	4
Unit I	Spectroscopy-3			
Unit II	Photochemistry 2			
Unit III	Electrochemistry 2			
Unit IV	Quantum Chemistry 3			
Unit V	Thermodynamics 3: Irreversible Thermodynamics			
<b>CEM-403I</b>	Inorganic Chemistry Special - II	40+10	70	4
Unit I	Nanomaterials			
Unit II	Inorganic Solid Materials			
Unit III	Inorganic Photochemistry			
Unit IV	Physical Characterization of Inorganic Compounds-III			
Unit V	Synthetic Methodology for Transition and Non-transition Metal Complexes			
CEM-403O	Organic Chemistry Special - II	40+10	70	4
Unit I	Asymmetric synthesis			
Unit II	Nucleoside and nucleotide and Nucleic acids			
Unit III	Bioorganic chemistry			
Unit IV	Reaction Intermediates			
Unit V	Natural product 2			

CEM-403P	Physical Chemistry Special II	40+10	70	4
Unit I	Photophysical processes			
Unit II	Instrumental Methods of Chemical Analysis			
Unit III	Advanced Materials			
Unit IV	Statistical thermodynamics			
Unit V	Biophysical Chemistry			
CEM-404	Grand Viva	50	70	4
CEM -495	Project (Inorganic/ Organic/ Physical)	50	90	4
CEM -496	Internship	50	90	4
	Total Marks	300		
	Total Credit			24

#### **SEMESTER-I**

CEM-101: Inorganic Chemistry General I Marks: 50 Credits: 4 Classes: 70L

#### Unit-01

## Selected Topics on the Chemistry of s- and p- Block Elements

Structure and bonding in higher boranes based on Lipscomb's topological concept, styx and Wade's rules, borohydride, B H <sup>2-</sup> anions, metalloboranes, carboranes and other heteroboranes, reactions of boron hydrides, frustrated Lewfs pair; alkali metal complexes with macrocyclic ligands (crown ethers, cryptates, spherand, ionophores); aqueous and complex chemistry of beryllium and aluminium, basic beryllium compounds; compounds of noble gases and their uses as ligands; main group organometallics.

## Unit-02

## **Coordination Chemistry I**

Crystal field theory (CFT), limitations, adjusted CFT; splitting of d-orbitals in linear, triangular, tetrahedral, square planar, trigonal bipyramidal, square pyramidal, octahedral and cubic fields of similar and dissimilar ligands; CFSEs in weak/strong field environments, spinel and inverse spinel complexes, octahedral site preference energy, tetragonal distortion and Jahn-Teller effect, static and dynamic Jahn-Teller; effect of crystal field stabilization on ionic radii, lattice energy, hydration enthalpy and stability of complexes (Irving-Williams order), kinetic aspects of crystal field stabilization, crystal field activation energy, labile and inert complexes.

## Unit-03

## **Environmental Chemistry**

Photochemical smog and mechanism of formation; chemistry of stratospheric ozone depletion, formation of Antarctic ozone hole and acid rain and their consequences; monitoring/determination of atmospheric pollutants; major water pollutants, biodegradation of organic matters, nutrients in aquatic ecosystem, BOD and COD and their determinations; chemical speciation of different elements in aquatic environment, ground water pollution due to arsenic and heavy metals; eutrophication, waste water and its control; determination of inorganic/organic pollutants in waste water; soil pollution due to pesticides, herbicides, fertilizers, plastics, radioactive waste, E-waste, bio-/nonbio- degradable pollutants; greenhouse gases, global warming, carbon sequestration.

## Unit-04

## **Nuclear Chemistry**

Nuclear shell model, determination of spin parity, nuclear stability; artificial nuclear reactions: various important nuclear reactions, Bethe's notation of nuclear reactions, nuclear reactions versus chemical reactions; radioactive equilibrium and its types; Szilard-Chalmer's effect and its uses; nuclear fission: spontaneous fission, mechanism of nuclear fission, chain reactions; nuclear reactor, breeder reactor, neutron economy, four factor formula; fusion energy and artificial sun; radiochemical methods of analysis: neutron activation analysis, isotopic dilution analysis, analysis related to biological, medical and agriculture fields; interaction of radiation with matters; determination of structures and establishment of reaction mechanisms; radiopharmaceuticals, radiation hazards and safety measures.

#### Unit-05

## Organometallic Chemistry I

Definition and classification of organometallic compounds, application of 18-electron and 16-electron rules to transition metal organometallic complexes, isolobal and isoelectronic relationships; metal-alkyl, -allyl, -carbene, - carbonyl, -carbide and -cyclopentadienyl complexes; structure and bonding in  $\eta^2$ - ethylenic and  $\eta^3$ -allylic compounds with typical examples, heptacity, kinetic and thermodynamic stability of organometallic compounds; structure and bonding of

ferrocene, K[Pt(C<sub>4</sub>H<sub>4</sub>)Cl<sub>3</sub>], [(Ph<sub>3</sub>P)<sub>2</sub>Pt(Ph-C $\equiv$ C-Ph)]; reactions of organometallic complexes *e.g.*, substitution, oxidative addition, reductive elimination, insertion and elimination; electrophilic and nucleophilic reactions of coordinated ligands, fluxional organometallic compounds.

## **Course Outcome (C.O.):**

Unit 01: The students are expected to have the ability to understand (i) systematic understanding of the chemical reactivities of s and p-block elements, (ii) structure and bonding concepts in boranes, (iii) alkali metal complexes with macrocyclic ligands.

Unit 02: The students are expected to learn (i) the splitting of d orbitals in different fields, (ii) various theories of coordination compounds, (iii) Jahn - Teller affects, Irving-Williams order.

Unit 03: The students are expected to have the understanding on (i) the impact of different types of pollution, (ii) chemistry of air pollution in the troposphere and stratosphere, (iii) chemical speciation of different elements in aquatic environment.

Unit 04: The students will learn about in particular (i) nuclear properties and structure, radioactive equilibrium, and nuclear reactions, (ii) synthetic elements, nuclear energy, (iii) radiochemical methods of analysis, radiopharmaceuticals, radiation hazards

Unit 05: The students will learn about (i) properties and reactivities, (ii) structure and bonding, and (iii) principles of transition metal coordination complexes in understanding reactivities and properties of organometallic compounds.

## **Reference Books:**

- 1. J. E. Huheey, Inorganic Chemistry, 4th Ed, Pearson (2008).
- 2. N. C. Norman, Periodicity and the p-Block Elements, No.51, 2nd Ed, Oxford University Press (2010).
- 3. N. N Greenwood and A. Earnshaw, Chemistry of the Elements, Pergamon Publishing Ltd (1989).
- 4. P. Atkins, Inorganic Chemistry, 5th Ed, Oxford University Press (2010).
- 5. D. Ray, Coordination Chemistry, NPTEL Course Material; http://mplel.ac.in/courses/104105033/
- 6. R. Gopalan and V. Ramalingam, Concise Coordination Chemistry, Sangam Books Ltd (2001).
- 7. S.E. Manahan, Environmental Chemistry, 11<sup>th</sup> Ed, Lewis Publishers (2022).
- 8. A. K. De, Environmental Chemistry, 4th Ed, New Age International Publishers (2000).
- 9. J. Seinfeld and S. Pandis, Atmospheric Chemistry and Physics, 2<sup>nd</sup> Ed, Wiley (2006).
- 10. H.J. Arnikar, Essentials of Nuclear Chemistry, 4th Ed, New Age International Publications (2001).
- 11. G. Friedlander, J.W. Kennedy, E. S. Macias and J.M. Miller, Nuclear & Radiochemistry, 3rd Ed, John Wiley & Sons Inc (1981).
- 12. G. Choppin, J.-O. Liljenzin and J. Rydberg, Radiochemistry and Nuclear Chemistry, 2<sup>nd</sup> Ed, Elsevier (1995).
- 13. R. H. Crabtree, The Organometallic Chemistry of Transition Metals, Wiley (1998).
- 14. A. G. Samuelson, Introduction to Organometallic Chemistry; http://nptel.ac.in/courses/104108062/
- 15. B.D. Gupta and A. J. Elias and, Basic Organometallic Chemistry: Concepts, Syntheses and Applications of Transition Metals, Taylor and Francis (2010).

## CEM-102: Organic Chemistry General I Marks: 50 Credits:4 Classes:70L

## Unit-01

## **Electronic property of conjugated organic systems:**

MO treatment of acyclic and cyclic conjugated systems; Huckel's rule and concept of aromaticty; annulenes, heteroannulenes, fullerenes ( $C_{60}$ ), alternate and non-alternate hydrocarbons, anti-aromaticity, pseudo-aromaticity, homo-aromaticity; graphical methods - Frost diagram; Huckel treatment-applications to ethylene, allyl, cyclopropenyl, butadiene, cyclobutadiene;

Modern Aromaticity Concepts: Möbius aromaticity (beyond just mentioning it), Metalloaromaticity, Aromaticity in excited states (Baird's rule), 3D aromaticity (e.g., in fullerenes and boranes)

## Unit-02

## **Stereochemistry 1**

Static, Dynamic stereochemistry: Winstein-Holness equation, Curtin-Hammett principle; conformational analysis of cyclohexane, cyclohexenes (A1,2-strain), alkylidene cycloalkanes (A1,3-strain), cyclohexanone, 2-haloketone effects, 2-, 3-and 4-alkyl ketone effects, decalin and their derivatives; conformation and reactivity- of some acyclic and cyclic systems, Diastereoselective synthesis: Felkin-Anh, Prelog, Horeau, Cieplak and Zimmerman-Traxler Models in connection with addition reactions to carbonyl compounds.

#### Unit-03

## **Pericyclic reactions**

Classification and stereochemical modes, thermal and photo pericyclic reactions, selection rules, stereochemistry, reactivity, regioselectivity and periselectivity in cycloaddition reactions, electroreversion reactions, 2-component cycloadditions, Ionic cycloaddition reactions, dipolar cycloaddition reactions, introduction to Click chemistry, ene reaction, cheleotropic reactions, sigmatropic rearrangements, carbene addition; rationalization based on Frontier MO approach, correlation diagrams, Dewer-Zimmermann approach, Mobius and Huckel systems; Sommelet, Hauser, Cope and Claisen rearrangements, Ene reaction, Wittig rearrangement.

Pericyclic reactions in natural product synthesis (3 /4 examples).

#### Unit-04

## NMR spectroscopy & Mass spectrometry

Principle, instrumentation and different techniques (CW and FT) of NMR spectroscopy; factor influencing chemical shift, spin-spin interactions, coupling constant(J), spin decoupling, spin tickling; Discussion on ABX, AMX, ABC, A<sub>2</sub>B<sub>2</sub> in proton NMR, NOE, Dynamic NMR [variable temperature], equilibrium study; introduction to <sup>13</sup>C-NMR spectroscopy; application of NMR spectroscopy. and other spectroscopical techniques to simple structure and mechanistic problems. Working principle; ion generation: EI, CI, ion- detection, fragmentation, analysis, abundance; molecular ion, metastable, isotope peak; ion molecule interaction, fragmentation patterns analysis, McLafferty rearrangement; nitrogen rule; mass analysis and mass accuracy. Combined problems including UV-Vis, IR, NMR, Mass spectrometry.

## Unit-05

## Natural product -1

Terpenoids: Isoprene rule, structure elucidation (by chemical and spectroscopical methods), synthesis, biogenesis and biosynthesis of representative examples of acyclic, monocyclic and bicyclic monoterpenes.

Alkaloids: Classifications, familiarity with methods (chemical and spectroscopic) for structure elucidation, biosynthesis, synthesis and biological activity of alkaloids like nicotine, atropine, coniine and papaverine.

## **Course Outcome (C.O.):**

Upon successful completion of these courses, students will be able to:

Unit 01: Explain and utilize Huckel's, describe electronic features of conjugated organic compounds, understand and apply Hammett equation and its modifications to analyse and predict the effect of substituents on the reactivity and equilibrium of aromatic compounds.

Unit 02: Explain and apply Winstein-Holness to correlate reaction rate with conformational equilibrium, Curtin-Hammett principle to understand how the product distribution in a reaction is determined when the reacting conformations interconvert rapidly. Understand, apply different

models and predict stereochemical outcomes in the addition reactions to carbonyl compounds

Unit 03: Classify different types, Identify differentiate stereochemical modes and, understand Woodward-Hoffmann selection rules, Dewar-Zimmermann approach, Möbius and Hückel and apply them to determine feasibility of different modes including mechanism.

Unit 04: Explain the fundamental principles and Describe the instrumentation of NMR spectroscopy, Analyze and interpret spin-spin coupling, Understand and apply spin decoupling techniques, Classify spin systems in proton NMR, Provide an introduction of 13C.

Explain the working principle of mass spectrometry, Describe EI and CI, detection process, Explain the process of fragmentation of molecular ions, Identify and interpret molecular ion peak, metastable peaks, and isotope peaks, Analyze and interpret common fragmentation patterns of organic molecules. Utilize NMR and Mass to solve structure, to gain mechanistic insight.

Unit 05: State and apply isoprene rule, Describe and utilize chemical methods for the structure elucidation of terpenoids and alkaloids. Outline and discuss synthetic strategies, biogenesis and bisosynthesis of terpenoids. Classify alkaloids, Describe and apply various chemical methods used for the structure elucidation, Outline and discuss the biosynthetic pathways, Describe synthetic strategies, Summarize and discuss the known biological activities of nicotine, atropine, coniine and papaverine.

- 1. R. T. Morison, and R. N. Boyd, Organic Chemistry, 6th Edn, Prentice-Hall India Pvt Ltd, New Delhi, 1992.
- 2. F. A. Carey and R. J. Sundberg, Advanced Organic Chemistry Part A and Part B, 4th Edn, Plenum Press, New York, 2001.
- 3. W. J. I. Noble, Highlights of Organic Chemistry, Mercel Dekker, New York, 1974.
- 4. J. Clayden, N. Greeves, S. Warren and P. Wothers, Organic Chemistry, Oxford University Press, Oxford, 2001.
- 5. J. March, Advanced Organic Chemistry.
- 6. D. Nasipuri, Stereochemistry of Organic Compounds, 2nd Edn, Wiley Eastern, New Delhi, 1993.
- 7. E. L. Eliel, S.H. Wilen and L.N. Mander, Stereochemistry of Organic Compounds, John Wiley & Sons, New York, 1994.
- 8. R. S. Ward, Selectivity in Organic Synthesis, John Wiley & Sons, New York, 1999. F. A.
- 9. I. Fleming, Frontier Orbitals and Organic Chemical Reactions, John Wiley, New York, 1980.
- 10. R. B. Woodward and R. Hoffman, The Conservation of Orbital Symmetry, Verlag Chemie GmbH, 1970.
- 11. T. L. Gilchrist and R. C. Storr, Organic Reactions and Orbital Symmetry, 2nd Edn, Cambridge University Press, Cambridge, 1979.
- 12. E. R. Lehr and A. P. Merchand, Orbital Symmetry and Cyclo-addition, Academic Press, New York, 1972.
- 13. G. B. Gills and M. R. Willis, Pericyclic Reactions, Chapman and Hall, London, 1974.
- 14. R. E. Lehr and A. P. Marchand, Orbital Symmetry a Problem solving approach.
- 15. T. L. Gilchrist & R.C. Storr, Orbital Symmetry in Organic Reactions.
- 16. J. R. Dyer, Applications of Absorption Spectroscopy of Organic compounds, 2nd print, Prentice Hall, New Jersey, 1971.
- 17. W. Kemp, Organic Spectroscopy, 3rd Edn, McMillan, Hong Kong, 1991.
- 18. R. M. Silverstein and F. Webster, Spectrometric Identification of Organic Compounds, 6th Edn, John Wiley, New York, 1998.
- 19. D. H. Williams and I. Fleming, Spectroscopic Methods in Organic Chemistry, 5th Edn, Tata McGraw Hill, New Delhi, 2005.
- 20. D. L. Pavia, G. M. Lampman, G. S. Kriz and J. R. Vyvyan, Spectroscopy, Brooks/Cole, a part of Cengage Learning, 2008.
- 21. R. C. Banks, E.R. Matjeka and G. Mercer, Introductory Problems in Spectroscopy,

Benjamin/Cumings Publishing Co, 1980.

- 22. K. Biemann, Mass Spectrometry Application to Organic Chemistry, McGraw-Hill, New York, 1962.
- 23. H. Budzikiewicz, C. Djerassi and D.H. Williams, Mass Spectrometry of Organic Compounds, Holden Day, 1967.
- 24. J. Barker, Mass Spectrometry, 2nd Edn, John Wiley, New York, 2000.
- 25. C. Dass, An Introduction to Biological Mass Spectrometry, Wiley, New York, 2002.
- 26. K. Downard, Mass Spectrometry: A Foundation Course, Royal Society of Chemistry, UK, 2004.
- 27. G. Siurdek, The Expanding Role of Mass Spectrometry in Biotechnology, MCC Press, San Diego, 2004.
- 28. K. Nakanishi, T. Goto, S. Ito, S. Natori and S. Nozoe, Natural Products Chemistry, Vol I, Academic Press, New York, 1974.

## CEM-103: Physical Chemistry General I Marks: 50 Credits: 4 Classes: 70L

#### Unit-01

## **Quantum Chemistry-1:**

Schrödinger equation, Basic postulates and theorems, Physical interpretation of wave function, Stationary states, Operator formation, Atomic unit system, Heisenberg's equation of motion; Particle in a box problem, Finite barrier problem and tunnelling; Linear harmonic oscillator, Ladder operators, Angular momentum problem, Rigid rotor; The Hydrogen atom problem and its implications.

## Unit-02

## **Symmetry and Group theory-:**

Groups and their properties, Subgroups, Classes and the related theorems; Commutative (abelian) groups and cyclic groups and their examples; Group multiplication tables and the rearrangement theorem; Symmetry elements, Operations and their properties, Symmetry in platonic solids, Identification of point groups, Similarity transformation and the invariance of characters, Block diagonalization, Direct product of matrices and their characters etc; Matrix representation of symmetry operations, Characters of symmetry operations in a representation, Invariance of character under similarity transformation, The row / column orthogonality of characters, Reducible and irreducible representations, The "Great Orthogonality Theorem" (without derivation) and its corollaries.

## Unit-03

## **Spectroscopy-1:**

General introduction, nature of electromagnetic radiation, shapes & width of spectral lines, Intensity of spectral lines, Fourier transform; Understanding different spectroscopic techniques including UV-Vis; Morse potential energy diagram, bond dissociation energy.

*Microwave Spectroscopy*: Moment of Inertia and Classification of molecules, Diatomic molecule as rigid rotator, nonrigid rotator; Hyperfine Structures, Stark Effect and determination of Dipole moment.

*Infrared Spectroscopy*: Vibrational Spectra of diatomic Molecules, Harmonic Oscillator model, energy levels and selection rules; Anharmonicity and its effect on energy levels and spectral features, overtones and hot bands, vibration-rotation spectra of diatomic molecules, selection rules, P, Q and R branches; Group vibration, limitation of the concept, FTIR, NDIR techniques.

## Unit-04

## **Atomic Structure and spectroscopy:**

Bohr's theory of atomic structure, Sommerfield's modification, Zeeman Effect (normal and

anomalous) and fine structure; Vector model of atoms, Spin-orbit interaction, Coupling of angular momenta, Effect of high magnetic field, Lande g factor; Many-electron systems and Antisymmetry principle, atomic (and molecular) terms and fine structure.

## Unit-05

## **Photochemistry-1:**

Jablonski diagram, Fluorescence and phosphorescence, Kasha's Rule, Solvent effect on emission spectra, Stoke's shift; Photochemical laws, Quantum yield; Delayed fluorescence, Fluorescence quenching (dynamic and static), Stern - Volmer equation; Energy transfer (Forster's dipole coupling), Complex formation (excimer, exciplex); Nonradiative intramolecular electronic transition, Internal conversion, Inter-system crossing, Crossing of potential energy surface (Franck-Condon factor), Adiabatic and non-adiabatic cross over, The basis of the selection rules, Selection rules for radiation less transitions; Photophysical kinetics of unimolecular processes.

## **Course Outcome (C.O.):**

After the completion of this course, students will build a strong foundation in quantum chemistry, symmetry, spectroscopy, atomic structure, and photochemistry—mastering the mathematical frameworks, molecular interactions, and excited-state dynamics that govern chemical behaviour at the quantum level.

## **Reference Books:**

- **1.** I. N. Levine *Quantum Chemistry*.
- **2.** F. A. Cotton *Chemical Applications of Group Theory.*
- **3.** C. N. Banwell and E. M. McCash *Fundamentals of Molecular Spectroscopy*.
- **4.** Atkins & Friedman's *Molecular Quantum Mechanics*.
- **5.** G. Aruldhas *Atomic and Molecular Spectroscopy*.
- **6.** K. K. Rohatgi-Mukherjee *Fundamentals of Photochemistry*.
- 7. P. W. Atkins Physical Chemistry (Latest editions co-authored with Julio de Paula and James Keeler).

## CEM-194: Inorganic Chemistry Practical I Marks: 50 Credits: 4 Classes: 90 L

- I. Identification of inorganic salts by semi-micro qualitative analysis
- II. Quantitative analysis of metal ions in real samples such as ore/minerals, alloys, soil, natural water etc.

## **Course Outcome (C.O.):**

The students will have hands-on training on (i) qualitative identification of different cations and anions in a semi-micro scale, use of spot reagents and spot tests; (ii) dissolution of real samples like minerals, ores, alloys, biological samples by classical and green processes using ultrasound/microwave radiation,(iii) quantitative estimation of major /minor constituents and also water quality analysis.

- 1. A. I. Vogel, A Textbook of Macro and Semimicro Qualitative Inorganic Analysis, 4th Ed, Longmans Green and Co (1955).
- 2. Vogel's Textbook of Quantitative Inorganic Analysis including Elementary Instrumental Analysis, John Bassett Publisher (1978).
- 3. H.M. Kingston and L. B. Jassie, Introduction to Microwave Sample Preparation: Theory and Practice, ACS Professional Reference Book (1988).

## **CEM-195: Organic Chemistry Practical I**

- (a) Identification of organic compounds by systematic qualitatitve analysis
- (b) Spectroscopic Analysis of Organic Compounds:
- (i) assignment of labeled peaks in the 1H NMR spectra of the known organic compounds and explain the relative  $\delta$ -values and splitting pattern.

Marks: 50

Credits: 4

Classes: 90 L

(ii) assignment of labeled peaks in the IR spectrum of the same compound

The students must record full spectral analysis of at least 15 (fifteen) compounds from the following list:

- (a) 4-Bromoacetanilide; (b) 2-Bromo-4'-methylacetophenone; (c) Vanillin; (d) 2-Methoxyacetophenone; (e) 4-Aminobenzoic acid; (f) Salicylamide; (g) 2-Hydroxyacetophenone; (h) 1,3-Dinitrobenzene; (i) Benzyl acetate; (j) trans-4-Nitrocinnamaldehyde; (k) Diethyl fumarate;
- (l) 4-Nitrobenzaldehyde; (m) 4-Methylacetanilide; (n) Mesityl oxide; (o) 2-Hydroxybenzaldehyde;
- (p) 4-Nitroaniline; (q) 2-Hydroxy-3-nitrobenzaldehyde; (r) 2,3-Dimethylbenzonitrile; (s) Pent-1-yn-3-ol; (t) 3-Nitrobenzaldehyde; (u) 3-Ethoxy-4-hydroxybenzaldehyde; (v) 2-Methoxybenzaldehyde; (w) Methyl 4-hydroxybenzoate; (x) Methyl 3-hydroxybenzoate; (y) 3-Aminobenzoic acid; (z) Ethyl 3-aminobenzoate; (aa) Ethyl 4-aminobenzoate; (bb) 3 Nitroanisole; (cc) 5-Methyl-2-nitroanisole; (dd) 3-Methylacetanilide

## **Course Outcome (C.O.):**

Upon successful completion of these courses, students will be able to: apply the knowledge of qualitative analysis and identify simple organic molecules, Interpret and predict 1H-NMR Spectra of simple organic molecules, analyse IR spectra.

## **Reference Books:**

## **SEMESTER-II**

## CEM-201: CBCS-I (Fundamentals of food and drugs) Marks: 50 Credits:4 Classes:70L

## Unit-01

#### **Constituents of Food:**

Water: Water in foods and its properties,

Carbohydrates: Sources and physicochemical and functional properties,

Proteins: Sources and physico-chemical and functional properties, Purification of proteins, Common food proteins,

Lipids: Sources and physico chemical and functional properties, PUFA (Polyunsaturated Fatty Acids), Lipids of biological importance like cholesterol and phospholipids, Hydrogenation and rancidity of lipids, Saponification number, iodine value of lipids,

Vitamins and Minerals: Sources, classification and structures of minerals & vitamins, Effect of processing and storage of vitamins, Pro vitamins A & D; Vitamins as antioxidants

Food Pigments & Flavouring Agents: Importance, types and sources of pigments, their changes during processing and storage

## Unit-02

## Introduction to food microbiology:

Introduction to food microbiology- definition, historical development and significance, Factors influencing the growth and survival of microorganisms in foods, Role of microbes in fermented foods and genetically modified foods, Food spoilage, Types and causes of food spoilage.

Microbiology of milk & milk products like cheese, butter, ice-cream,

Microbiology of meat, fish, poultry & egg and their products, Microbiology of cereal and cereal products like bread, confectionary etc.

#### Unit-03

## **Food preservation:**

Principles and methods: Canning; Preservation principle of canning of food items, thermal process time calculations for canned foods, spoilage in canned foods; Dehydration and drying of food items; Water activity of food and its significance in food preservation, IMF, Low temperature preservation; freezing and cold storage, cold chain, Preservation by fermentation; curing and pickling, Use of preservative in foods; chemical preservative, biopreservatives, antibiotics, lactic acid bacteria, Hurdle technology.

#### Unit-04

## **Basic principle of Pharmacology:**

Introduction to Pharmacology: Definition and scope of pharmacology, Drug nomenclature (chemical, generic, trade names), Sources of drugs, Drug regulation and approval processes (brief overview).

Pharmacokinetics: What the Body Does to the Drug; Absorption, Distribution, Metabolism (Biotransformation), Excretion:

Pharmacodynamics: What the Drug Does to the Body: Drug-receptor interactions, agonist, antagonist.

Routes of Drug Administration: Enteral routes (oral, sublingual, rectal), Other routes (topical, inhalation)

Introduction to major drug categories (e.g., analgesics, antibiotics, cardiovascular drugs - very brief overview of each)

## **Course Outcome (C.O.):**

Identify the chemical composition of food and how these constituents contribute to the nutritional, functional, and sensory properties. Identify and understand the diverse roles of microorganisms in food, both positive and negative, and the principles underlying food safety and preservation. Understand the effectiveness of different preservation methods and their impact on nutritional quality and safety of food product. Define basic pharmacological terms and concepts, differentiate between pharmacokinetics and pharmacodynamics, describe ADME, recognize major drug categories, different route of drug administration.

## **Reference Books:**

1. Introduction to medicinal chemistry-by G. L. Patrick

## CEM-202: Inorganic Chemistry General II Marks: 50 Credits: 4 Classes: 70L

## Unit-01

## **Selected Topics on the Chemistry of d- Block Elements**

Periodicity/aperoiodicity and diffusion cartograms; common/uncommon oxidation states; aqueous, redox and coordination chemistry; horizontal and vertical trends in respect of 3d, 4d, 5d elements with reference to Ti-Zr-Hf, V-Nb-Ta, Cr-Mo-W, Mn-Tc-Re and Pt group metals; iso- and heteropolyoxometalates with special reference to V, Mo, W: typical syntheses, reactions,

structures, applications; metal-metal bonded dinuclear d-metal complexes *e.g.*, dirhenium complexes; specific compounds like molybdenum bronze, tungsten bronze, Creutz-Taube ion, ruthenium red, Vaska complex, Magnus' green.

## Unit-02

## **Coordination Chemistry-II**

Metal-centered electronic spectra of transition metal complexes; microstates, Russel-Saunder's terms, determination of ground and excited state terms of  $d^n$  ions, splitting of  $d^n$  terms in  $O_h$  and  $T_d$  fields, colour and spectra, Tanabe Sugano and Orgel diagrams, hole formalism – inversion and equivalence relations, selection rule for spectral transitions, d-d spectra and CF- parameters, nephelauxetic series; magnetic properties of coordination compounds: spin and orbital moments, spin-orbit coupling, quenching of orbital moment, spin only formula, room- and variable-temperature magnetic moments.

## Unit-03

## **Complexes in Aqueous Solutions**

Stability of mononuclear, polynuclear and mixed ligand complexes in solutions, stepwise and overall formation complexes and their relations, trends in stepwise formation constants, statistical and non-statistical factors influencing stability of complexes in solution; stability and reactivity of mixed ligand complexes with reference to chelate effect and thermodynamic considerations; chelate, macrocyclic and template effects; metal ligand stability constant and its controlling factors, different methods (pH-metric, spectrophotometric) for measuring stability of complexes, calculations and determinations of composition (Job, mole-ratio and slope- ratio methods), evaluation of thermodynamic parameters.

#### Unit-04

## **Chemical Bonding**

Valence bond theory (VBT) and its application to H<sub>2</sub> molecule, concept of hybridization and resonance; salient of VBT and molecular orbital theory (MOT), LCAO MO theory; MOT of bonding in homonuclear and heteronuclear diatomic molecules of second period of periodic table, bonding in triatomic (H<sub>3</sub><sup>+</sup>, BeH<sub>2</sub>, H<sub>2</sub>O), polyatomic (BH<sub>3</sub>, NH<sub>3</sub>, CH<sub>4</sub>); MO diagrams, Walsh diagrams, structural geometry predictions: VSEPR and hybridization models, Bent's rule; application of VBT on H<sub>2</sub> molecule.

## Unit-05

## **Errors in Chemical Analyses**

Some important terms, systematic and random errors and their statistical treatment, standard deviation of calculated results; reporting computed data – significant figure convention, rounding data; statistical data treatment and evaluation – confidence intervals; null hypothesis and significance testing *e.g.*, Q-test, F-test, t-test; analysis of variance, detection of gross errors; sampling, standardization, calibration and linear regression, correlation coefficient, method of least squares – use of Excel to do least squares; errors in external standard calibration -- solvent blank, reagent blank; multivariate calibration, quality control, chemometrics; analytical figures of merit, sensitivity, detection limit; Lab-on-a-Chip.

## **Course Outcome (C.O.):**

Unit 01: The students are expected to gain knowledge in understanding (i) structure and bonding concepts in chemistry of d- block elements, (ii) chemical reactivities of different group trio-elements, (iii) metal -metal bonding in dinuclear d-metal complexes and bonding in polyoxometalates .

Unit 02: The learners are expected to be familiar with (i) splitting of d<sup>n</sup> terms in different fields, (ii) d-d spectra, (iii) magnetic properties of coordination compounds.

Unit I03: The students an expected to understand (i) stepwise and overall formation complexes

and their relations, (ii) stability and reactivity of metal-ligand complexes, (iii) Bjerrum method in the determination of stability constants and Job's method in evaluating composition.

Unit 04: The students are expected to understand nature of chemical bonding in (i) molecular species in the light of MOT, (ii)  $H_2$  molecule in the light of VBT, (iii) structural geometry predictions

Unit 05: The students are expected to have ideas of (i) error, accuracy and precision of chemical analysis, (ii) methods of statistical evaluation of data and reporting analytical data, (iii) regression and correlation analysis.

#### **Reference Books:**

- 1. J. E. Huheey, Inorganic Chemistry, 4th Ed. Pearson (2008).
- 2. N. N Greenwood and A. Earnshaw, Chemistry of the Elements, Pergamon Publishing Ltd (1989).
- 3. J.D. Lee, Concise Inorganic Chemistry, 5<sup>th</sup> Ed, Wiley India (P) Ltd (1996).
- 4. P. Atkins, Inorganic Chemistry, 5th Ed, Oxford University Press (2010).
- 5. D. Ray, Coordination Chemistry, NPTEL Course Material, http://nptel.ac.in/courses/104105033/
- 6. R. Gopalan and V. Ramalingam, Concise Coordination Chemistry, Sangam Books Ltd (2001).
- 7. A. E. Martell and R.D. Hancock, Metal Complexes in Aqueous Solutions, Springer Science (1996).
- 8. M. T. Beck, Chemistry of Complex Equilibria, Revised Ed, Halsted Press (1990).
- 9. D. A. Skoog, D. M. West, F. J. Holler, S. R. Crouch, Fundamental Analytical Chemistry, 8<sup>th</sup> Ed., Thomson (2004)
- 11. G. Frenking and S. Shaik (Eds), The Chemical Bond: Fundamental Aspects of Chemical Bonding, Wiley VCH (2014).
- 12. J. R. Lalane, Electronic Structure and Chemical Bonding (1996); <a href="https://doi.org/10.114213105">https://doi.org/10.114213105</a>
- 13. D. Brown, The Chemical Bond in Inorganic Chemistry: The Bond Valence Model, 2<sup>nd</sup> Ed, International Union on Crystallography (2016).
- 14. J. Kotecha, Errors and Statistics in Chemical Analysis, Lambert Academic Publishing (2012).
- 15. R. A. Day and A.L. Underwood, Quantitative Analysis, 6th Ed, Pearson (2022).
- 16. K. Weltner, Theory of Errors, Springer (2009).

## CEM -203: Organic Chemistry General II Marks: 50 Credits:4 Classes:70L

## Unit 01

## **Reagents and rearrangement reactions:**

Hydride transfer reagent - trialkylborohydrides, diimide, trialkyltin hydride, DIBAL, Na(CN)BH<sub>3</sub>; azobisisobutyronitrile (AIBN), Hypervalent iodine, Hinsberg reagent, Ley–Griffith reagent (TPAP), Petasis reagent; DCC, PCC, PDC, CuI, TEMPO-mediated reactions, Tebbe reagent.

Baker Venkata Raman, Brook, Neber, Sommelet-Hauser rearrangement, Meyer-Schuster rearrangement, Rupe rearrangement, Eschenmoser fragmentation, Eschenmoser-Claisen, Ferrier rearrangement.

#### Unit-2

## Heterocyclic chemistry-1

Small ring heterocyclic chemistry: Aziridines, azetidines (with application in medicinal chemistry. Different synthetic methods, characteristic reactivity including regioselctivity of pyrazole, imidazole, oxazole, thiazole, isooxazole, and their applications including the designing synthetic strategies of natural products, pharmaceuticals, and materials. Green synthetic methods for heterocycles including one-pot synthesis.

## Unit-3

## Logic in organic synthesis

Retrosynthetic analysis, disconnection approach, typical examples to illustrate the disconnection approach, functional group interconversion, umpolung, convergent synthesis. Total Syntheses as Case Studies; Introduction to automated synthesis and machine-assisted retrosynthesis tools; Baldwin's rule for ring closure reactions.

## Unit-4

## Organo-boron,-phosphorus and -sulfur, Basics of transition metal based organometallics

Chemistry of organoboron compounds, carboranes, hydroboration, Boronic esters, MIDA boronates, reactions of organoboranes, unsaturated hydrocarbon synthesis, allyl boranes, boron enolates; chemistry of organophosphorus compounds, phosphorus ylides, environmentally benign organophosphorus reagents; chemistry of organosulphur compounds, sulphur-stabilized anions and cations, sulphonium salts, sulphonium and sulphoxonium ylides.

Basics of transition metal based organometallics: Formalism and bonding, 18 el rules, Davies rule in connection with substitution and addition reaction.

## Unit-5

## **Photochemistry**

Basic principles, Jablonski diagram, photochemistry of olefinic compounds, Cis-trans isomerization, Photochemistry of ketones and unsaturated ketones, Paterno-Buchi reaction, Norrish type-I and -II reactions, photoreduction of ketones, di-pi-methane rearrangement, Barton reaction, Hofmann-Loeffler-Freytag reaction, photochemistry of arenes, photoreaction in solid state, method of generation and detection (ESR), radical initiators, reactivity pattern of radicals, substitution and addition reactions involving radicals, synthetic applications; cyclisation of radicals.

Modern Photochemistry: Photoredox catalysis and Hydrogen atom transfer reagents using visible light; Use of Ru, Ir complexes, or organic dyes as photocatalysts; Applications in C–H activation, cross-coupling, and green synthesis

## **Course Outcome (C.O.):**

Upon successful completion of these courses, students will be able to:

Unit 01: Identify, Understand and explain the mechanisms of wide range of important rearrangement and TEMPO mediated reactions, Predict the products of these reactions.

Unit 02: Describe synthesis and reactivity of pyridine, quinoline, isoquinoline, indole, pyrazole, imidazole, oxazole, thiazole, isooxazole, design synthetic strategies of natural products, pharmaceuticals, and materials.

Unit 03: Define and explain principles of retrosynthetic analysis, Apply the disconnection approach to simplify complex target molecules into readily available starting materials, Explain and apply the concept of umpolung and FGI, Design convergent synthetic strategies for complex molecules.

Unit 04: Describe the bonding and structure organoboron, Explain the hydroboration reaction and its stereochemical and regiochemical outcomes, Predict the products of various reactions of organoboranes, including oxidation, protonolysis, halogenation, and transmetalation, Describe the structure and bonding of organophosphorus compounds, explain different reaction of organophosphorus compounds, Describe the formation and stability, chemical reactivity of organosulphur compounds.

Unit 05: Explain the basic principles of photochemistry and photophysical processes, Interpret and utilize the Jablonski diagram, Describe the photochemistry of olefins arenes, Explain the mechanism and predict the products of Paterno-Buchi reaction, Norrish type-I and type-II reactions,  $di-\pi$ -methane rearrangement,

Explain the methods of generation and detection of radicals, identify common radical initiators,

Predict the products in different organic reactions involving radicals.

## **Reference Books:**

- 1. H. O. House, Modern Synthetic Reactions, 2nd Edn, Benjamin, 1971.
- 2. W. Caruthers, Modern Methods of Organic Synthesis, 3rd Edn, Cambridge University Press, Cambridge, 1996.
- 3. J. March, Advanced Organic Chemistry Mechanism and Structure in Organic Chemistry.
- 4. Herbert C. Brown, Organic Syntheses via Boranes, John Wiley and Sons, New York, 1975.
- 5. H. C. Brown, A. Pelter, K. Smith; Jonathan Clayden, Nick Greeves, and Stuart Warren. "Organic Chemistry," Oxford University Press, 2014.
- 6. Lowry and Richardson, Mechanism and Theory in Organic Chemistry, (Harper Row Publishers, New York).
- 7. J. A. Joule, K. Mills, Heterocyclic Chemistry, 5th Edn, John Wiley & Sons Ltd, UK, 2010.
- 8. R. Kartritzky, Handbook of Heterocyclic Chemistry, Pergamon Press, London, 1986.
- 9. R. R. Gupta, M. Kumar, V. Gupta, Heterocyclic Chemistry II, Springer Pvt Ltd, India, 2005.
- 10. R. K. Bansal, Heterocyclic Chemistry, 4th Edn, New Age International (P) Ltd, India, 2005.
- 11. T.L. Gilchrist, Heterocyclic Chemistry, 3/e, Pearson; Heterocyclic Chemistry by A R Katrizsky
- 12. J. H. Fuhrhop and G. Li, Organic Synthesis, Concepts and Methods, Wiley-VCH, New York, 2003.
- 13. S. Warren, Organic Synthesis The Disconnection Approach.
- 14. S. Warren, Designing Organic Synthesis Tactics of Organic Synthesis.
- 15. T.-L. Ho; Stuart Warren and Paul Wyatt, Organic synthesis, the disconnection approach, 2nd edition, Wiley, 2012.
- 16. G. H. Whitham, Organosulphur Chemistry, Oxford Chemistry Primers series.
- 17. O. L. Chapman, Some Aspects of Organic Photochemistry, Dekker, 1967.
- 18. J. M. Coxon and B. Halton, Organic Photochemistry, Cambridge University Press, Cambridge, 1974.
- 19. R. O. C. Norman and J. M. Coxon, Principles of Organic Synthesis, 3rd Edn, ELBS, 2003.
- 20. J. Singh and J. Singh, Photochemistry and Pericyclic Reactions, 3rd Edn, New Age International (P) Ltd, India, 2012.
- 21. A. Griesbeck, M. Oelgemoller and F. Ghetti, Organic Photochemistry and Photobiology, 3rd Edn, Vol I, CRC Press, Boca Raton, FL, 2012.
- 22. N. J. Turro, Molecular Photochemistry, Benjamin and Co, 1955.
- 23. W. A. Noyes, G.S. Hammond and J. N. Pitts, Advances in Photochemistry, Vol I, Interscience Publisher, New York, 1964.
- 24. D. C. Neekers, Mechanistic Organic Photochemistry, Reinhold, New York, 1967.
- 25. J. M. Coxon and B. Halton, Organic Photochemistry, Cambridge University Press, Cambridge, 1974.
- 26. C. H. J. Wells, Introduction to M.L. Photochemistry, Chapman and Hall, London, 1974.
- 27. A. Griesbeck, M. Oelgemoller and F. Ghetti, Organic Photochemistry and Photobiology, 3rd Edn, Vol I, CRC Press, Boca Raton, FL, 2012.

## CEM -204: Physical Chemistry General II Marks: 50 Credits:4 Classes:70 L

#### Unit-01

## **Quantum Chemistry-2:**

The variational method, Eckart's theorem, Application of variational method to the Helium atom problem; Linear variational method, orbital and spin angular momenta; Chemical bonding in diatomic molecules, Elementary concepts of MO and VB theories, Hückel treatment for liner

conjugated hydrocarbon systems, charge density and bond order calculations; Perturbation theory (time independent nondegenerate), Application of nondegenerate perturbation theory to the Helium atom problem, Nondegenerate perturbation theory and its application to Zeeman and anomalous Zeeman effect; nonrigid rotor, anharmonic oscillator.

## Unit-02

## **Symmetry and Group theory-2:**

Quantum mechanics and group representation theory, Direct product representation, the "Great Orthogonality Theorem" (without derivation) and its corollaries, character tables, Vanishing of quantum mechanical integral, Transition probability, Selection Rules, Projection operation, Symmetry adapted linear combination of atomic orbitals; Application of group theory to Ligand and crystal field theory: Splitting of orbitals and free ion terms in weak crystal fields, symmetries and multiplicities of energy levels in strong crystal fields, Correlation diagram, MO treatment of large molecules with symmetry.

#### Unit-03

## **Chemical Kinetics-1:**

Theories of reaction rates, Collision theory, Transition state theory, Arrhenius equation and the activated complex theory, activation energy, Potential energy surface – analysis of molecular geometry and chemical reaction dynamics, reaction coordinates and reaction paths, saddle point; Calculation of potential energy- simple ideas of ab-Initio and semi-empirical methods, BEBO method; Transition state theory and thermodynamics, Absolute rate theory, sample case studies, comparison with collision theory; Ionic reactions in solution: effect of dielectric constant and ionic strength, Enzyme catalysis and Enzyme inhibition reactions, Oscillating reaction, Kinetics of polymerization reactions.

## Unit-04

## **Chemical Thermodynamics-1:**

Mathematical and thermodynamic probability, Entropy and probability, Boltzmann-Planck equation, Partial molar properties (partial free energy, molar volume and molar heat content), their significance and determination; Free energy of a mixture, Partial molal quantities, Analytical form of the chemical potential in ideal solutions, Chemical potential of a solute in a binary solution; Application of Gibbs Duhem equation, Nonideal solutions, concept of fugacity/activity: experimental determination of activity coefficients of non-electrolytes; Application of thermodynamics to micelles and microemulsion.

#### Unit-05

## **Solid state Chemistry:**

Defects in solids, line and plane defects; Determination of equilibrium concentration of Schottky and Frenkel defects, Stoichiometric imbalance in crystals and non-stoichiometric phases, Colour centres in ionic crystals; Band theory, Band gap, Metals, Insulators, Semiconductors (intrinsic and extrinsic), Hopping semiconductors, Rectifiers and transistors; Bonding in metal crystals: Free electron theory, Electronic specific heat, Hall effect, Electrical and thermal conductivity of metals, Superconductivity and Meissner effect; Organic conducting solids, Solid state reactions; Applications of semiconductors in catalysis, Energy conversion and environment remediation.

#### **Course Outcome (C.O.):**

After the completion of this course, students will advance their understanding of quantum chemistry, group theory, kinetics, thermodynamics, and solid-state chemistry—mastering methods like variational and perturbation theory, symmetry-driven orbital analysis, reaction dynamics, entropy and chemical potential in real systems, and the electronic structure and functional properties of solids.

#### **References Books:**

- **1.** I. N. Levine *Quantum Chemistry*.
- **2.** F. A. Cotton *Chemical Applications of Group Theory.*
- **3.** K. J. Laidler *Chemical Kinetics*.
- **4.** P. W. Atkins & Julio de Paula *Physical Chemistry*.
- **5.** A. R. West *Solid State Chemistry and Its Applications.*
- **6.** S. Glasstone *Thermodynamics for Chemists*.
- 7. M. S. Ramachandra Rao & Shubra Singh *Solid State Physics and Chemistry*.

## **CEM-295: Inorganic Chemistry Practical II**

I. Synthesis and characterization of coordination compounds

II. Separation of binary metal ion mixtures by solvent extraction, ion exchange column followed by estimation of the constituents.

Marks: 50 Credits: 4 Classes: 90 L

Marks: 50 Credits: 4 Classes: 90 L

## **Course Outcome (C.O.):**

The students are expected to (i) acquire the knowledge and skills required to plan inorganic complex compound synthesis followed by assay of the metal ion, (ii) develop methods for the separation of binary mixtures using solvent extraction and determination of the metals, (iii) ion exchange column separation followed by estimation of the constituents.

#### **Reference Books:**

- 1. A. J. Elias, A Collection of Interesting General Chemistry Experiments, Universities Press (India) Pvt Ltd (2002).
- 2. Vogel's Textbook of Quantitative Inorganic Analysis including Elementary Instrumental Analysis, John Bassett Publisher (1978).
- 3. G. N. Mukherjee, Advanced Experiments in Inorganic Chemistry, U.N. Dhar & Sons Pvt Ltd(2010).

## **CEM-296: Physical Chemistry Practical I**

- 1. Studies on the kinetics of iodination of acetone.
- 2. Determination of solubility product of PbI<sub>2</sub> by titrimetric method.
- 3. Determination of coordination number of Cu<sup>2+</sup> (partition method).
- 4. Ion exchange capacity of resin.
- 5. Verification of Beer's law and studies on the kinetics of alkaline hydrolysis of crystal violet.
- 6. Conductometric titration of a mixture of acids.
- 7. Estimation of concentration of a mixed acid (mixture of a strong and a weak acid) pH-metrically.
- 8. Studies on alkali hydrolysis of ethyl acetate conductometrically.

## Course Outcomes (C.O.): Reference Books:

## **SEMESTER-III**

CEM-301: CBCS-II (Building Materials, Medicinal Plants and Polymers)

Classes: 70 L

## Unit-01

## **Building materials:**

Cement: Manufacturing process, key ingredients and their roles, hydration process of cement, setting time, and their significance, types of cement and their common applications, properties of fresh and hardened concrete related to cement.

Brick: Illustrate Physical steps and chemical changes in the brick formation process; key raw materials, important properties of good quality bricks, different types of bricks and their typical uses.

Fly ash bricks (containing class C and class F fly ash): Fly ash chemistry is highly interesting and can be used making bricks, concrete and cement products, road construction.

Floor tiles: Ceramic tiles, vitrified tiles, stone tiles, resilient flooring, epoxy morter and grout.

Wall Paints:

Pigments- Dioxazine violet; Binders (Resin)- Acrylics; Solvents- Tolune, Xylene; Pigments- TiO<sub>2</sub>, Fe<sub>2</sub>O<sub>3</sub>, Cr<sub>2</sub>O<sub>3</sub>, ultramarine blue; Fillers/Extenders- Quartz sand, Talc, Keoline clay.

Solar Energy for household purposes

#### Unit 02

#### **Common Medicinal Plants and Their Active Constituents:**

Medicinal plants, Historical and cultural significance, Commonly used medicinal plants in traditional systems (e.g., Ayurveda, local traditions), Nomenclature (common and scientific names), Basic plant morphology relevant to identification.

Discuss Traditional uses, major active constituents, general pharmacological activities, and preparation (remedies) of medicinal plants that include but are not limited to the following plants.

Tulsi (Holy Basil - *Ocimum sanctum/tenuiflorum*) Traditional uses, major active constituents (eugenol, ursolic acid, rosmarinic acid), general pharmacological activities (adaptogenic, anti-inflammatory), Ginger (*Zingiber officinale*), Turmeric (*Curcuma longa*), Ashwagandha (*Withania somnifera*), Neem (*Azadirachta indica*)

#### Unit 03

## **Introduction to Polymer chemistry:**

Definition, natural vs synthetic, monomers and polymerization, Nomenclature and Classifications, Degree of polymerization and its significance, Molecular Weight and Distribution, PDI, Polymerization Reactions: Addition vs Condensation Polymerization, step-growth vs chain-growth mechanism.

Applications of synthetic polymers: LDPE, HDPE, polypropylene, polyvinyl chloride (pvc), polyamides (nylon), polycarbonates, elastomers (rubbers, silicones), fibers (e.g., aramids).

#### Unit 04

## Natural and semi-synthetic Carbohydrate Polymers:

Definition of polysaccharides, Distinction between homopolysaccharides and heteropolysaccharides. Degree of Polymerization (DP) in Polysaccharides.

Structure and properties of Natural Carbohydrate Polymers: Storage Polysaccharides: Starch and Glycogen; Structural Polysaccharides: Cellulose: Chitin:

Brief overview of gums, hyaluronic acid, heparin and their applications.

Production properties and applications of Semi-Synthetic Carbohydrate Polymers: Cellulose acetate, Cellulose nitrate, Methylcellulose (MC) and Carboxymethylcellulose (CMC), Chitosan.

## **Course Outcome (C.O.):**

Realization the fundamental aspects of cement and brick as essential building materials. Costs of flyash bricks are 20% less than traditional bricks, less load, less breakage during transport, use mortar

requirement reduce by 50% high fire resistance, no soaking of bricks in water, gypsum plaster can be applied directly. Above all, it is associated with solid waste management and avoidance of surface soil.

Explore commonly used medicinal plants and the key active constituents responsible for their therapeutic properties.

Identification, differentiate between natural and synthetic polymers, Identify and describe the key characteristics and applications of common synthetic polymers.

Understand the basic structure of the natural polymers (starch, glycogen, cellulose, chitin, pectin), Discuss the properties and applications of important semi-synthetic carbohydrate polymers from cellulose and starch (e.g., cellulose acetate, CMC, modified starches, chitosan).

## **Reference Books:**

- 1. S.K. Duggal, Building Materials.
- 2. P.C. Varghese, Building Materials.
- 3. K. K. Kar, Handbook of Flyash, Butterworth-Heinemann Inc. (2021).
- 4. Books Ceramic tile floors; https://www.researchgate.net
- 5. G. P. A. Turner, Chapman & Hall, Introduction of Paint Chemistry and Principles of Paint Technology (1997).
- 6. Camden Judy, A Guide to Common Medicinal Herbs: Herbal Medicine for Beginners Kindle Edition.
- 7. Healing Herbs, A beginner's guide to identifying, foraging, and using medicinal plants.
- 8. Tina Sams, Handbook of medicinal herbs by James A. Duke
- 9. Gauri Shankar Misra, Introductory Polymer Chemistry.

CEM 302: Inorganic Chemistry General III Marks: 50 Credits:4 Classes: 70 L

#### Unit-01

## Selected Topics on the Chemistry of f- Block Elements and Superheavy Elements:

Abundance, extraction, separation and recovery of lanthanoids; general electronic configuration; lanthanoid and actinoid contractions and consequences; relativistic effect, group characteristics and periodic trends, alloys and their uses; oxidation states; aqueous, redox, coordination and organometallic chemistry and comparison with d-block elements; comparison between lanthanoids and actinoids and their ion exchange separation patterns; lanthanoid compounds as high temperature superconductors, MRI and NMR shift agent, luminescentlanthanoids and antenna effect, solar photovoltaic cell; electronic, optical and magnetic properties,

Chemistry of superheavy elements, quest for superheavy elements and the limit of the periodic table.

#### Unit-02

## **Bioinorganic Chemistry-I:**

Role of metal ions, bioenergetic principle and role of ATP, ion pump: transport across biological membrane - Na<sup>+</sup>-K<sup>+</sup>- ATPase; metal ions transport and storage proteins: siderophore, ferritin, transferrin, ceruloplasmin; oxygen uptake proteins: myoglobin, haemoglobin, cooperative interaction, hemocyanin, hemerythrin, model synthetic dioxygen complexes; metalloenzymes, hydrolytic enzymes*e.g.*, carbonic anhydrase, carboxy peptidases, urease; redox enzymes*e.g.*, Fe-S proteins –ferredoxins; catalase, peroxidase, model studies, superoxide dismutases; ascorbic acid oxidase; metal ions toxicity and detoxification by chelation therapy.

#### Unit-03

## **Organometallic Chemistry II:**

Dewar-Chatt-Duncanson bonding model, Agostic interaction; catalysis by organometallic compounds; Wilkinson's catalyst, Tethered catalyst, Ziegler-Natta catalyst and Cossee-Arlman mechanism, Kaminsky catalyst; Tolman catalytic loop, syntheses gas - WGSR, hydroformylation, Monsanto acetic acid process, Wacker-Smidt process, C-H activation, CO<sub>2</sub> fixation, water oxidation, Cativa process, hydro-silation/phosphilynation/-amination/-cyanation reactions; synthetic gasoline - Fischer-Tropsch process and Mobil

process; polymerization, oligomerization and metatheses reaction of alkenes and alkynes, photodehydrogenation catalyst (platinum POP); metallo-fullerenes, bioorganometallics.

#### Unit-04

## Physical Characterization of Inorganic Compounds – I:

UV-Vis: Spectral analysis of inorganic, coordination and organometallic compounds, elementary idea on spectra of d<sup>n</sup> and f<sup>n</sup> ions; electronic transition time, designation of bands, effects of solvents, characteristic absorptions of varied chromophore systems, kinetics and mechanistic study; vibrational structures, selection rules and their violations, IR: Bonding and reaction pathways in inorganic, coordination and organometallic compounds; characteristic group frequencies: stretching and bending vibrations and their secondary shifts due to coordination, new bands upon coordination; characterization of varied geometrical and linkage isomers in different polyhedra; FTIR and interpretation of spectra.

NMR: <sup>1</sup>H NMR spectra ofdia- and paramagnetic inorganic, coordination and organometallic species; dipolarand contact shifts, magnetic susceptibility and resonance shifts; enumeration of antiaromatic, aromatic, quasiaromaic and super-aromatic systems; fluxionality, dynamic equilibrium, hapticity, probing chemical reactivity and reaction pathways; <sup>11</sup>B, <sup>13</sup>C, <sup>19</sup>F, <sup>31</sup>P, <sup>195</sup>Pt-NMR studies with suitable examples; 2D NMR, NMR shift reagent and MRI contrast agent.

#### Unit-05

## **Inorganic Reaction Mechanism:**

Mechanisms of substitution reactions in O<sub>h</sub> and sq planar d<sup>n</sup> ion complexes, associative, dissociative, interchange etc. pathways, solvent exchange, aquation, anation, base hydrolysis, acid-catalyzed aquation, pseudo-substitution; Eigen-Wilkins mechanism, Fuoss-Eigen equation, linear free energy relation, Hammett and Taft plots; nucleophilicity and rate scales, Gutmann donor number, Drago E & C scale; mechanisms of isomerization and racemization, Ray-Dutta/Bailar twist mechanism; stereospecificity, *cistrans*-effect, different theories and synthetic uses, *trans*- influence, stereoretentive/stereodynamic path;redox reactions: complementary and non-complementary, self-exchange; OSET/ISET mechanism; Franck-Condon barrier, potential energy diagram, redox catalyzed substitution reactions; Marcus theory, fast redox reactions in biological systems.

## **Course Outcome (C.O.):**

The students are expected to gain knowledge in understanding (i) electronic configuration, lanthanide/actinide contraction, oxidation states, reactivities etc. of f-block elements, (ii) comparison between lanthanoids and actinoids, (iii) quest for superheavy elements and limit for periodic table.

The students are expected to have ability of appreciate (i) chemistry of elements of life, role of metal ions in bioenergetics, transport and storage proteins, (ii) mechanism of the activity of oxygen uptake proteins, activity of the enzymes, (ii) toxic effects of metal ions and detoxification of by chelation therapy.

The students are expected to learn (i) design (ii) applications and (iii) special features of various organometallic compounds of transition metals including name catalysts.

The students are expected tounderstand the theoretical background various spectroscopic of techniques such as (i) UV-Vis, (ii) IR and FTIR, (iii) NMR and applying those spectroscopic methods as analytical tool in inorganic compounds.

The students will learnabout (i) stoichiometric/intimate reaction mechanisms;(ii) mechanisms of substitution, isomerization, racemization reactions; (iii) redox reactions, redox catalysed substitution reactions, fast redox reactions in biological system.

- 1. M. C. Aspinall, Chemistry of the f-Block Elements, Oxford University Press (2020).
- 2. F.A. Cotton, G. Wilkinson, C.A. Murillo and M. Bochmann, Advanced Inorganic Chemistry, 6th Ed, Wiley (2007).
- 3. M. Schadel and D. Shaughnessy, The Chemistry of Superheavy Elements, Latest Ed, Springer (2014).
- 4. G. N. Mukherjee and A. Das, Elements of Bioinorganic Chemistry, U. N. Dhur & Sons Pvt Ltd (2010).
- 5. D. Ray, Bioinorganic Chemistry, NPTEL Course Material, http://nptel.ac.in/courses/104105031/

- 6. S. J. Lippard and J. M. Berg, Principle of Bioinorganic Chemistry, University Science Books (1994).
- 7. R. H. Crabtree, The Organometallic Chemistry of Transition Metals, Wiley (1998).
- 8. A.G. Samuelson, Introduction to Organometallic Chemistry; http://nptel.ac. in /courses/104108662/
- 9. B.D. Gupta and A. J. Elias and, Basic Organometallic Chemistry: Concepts, Syntheses and Applications of Transition Metals, Taylor and Francis (2010).
- 10. C.N. Banwell, Fundamentals of Molecular spectroscopy, 4th Ed, McGraw Hill (2017).
- 11. A.B.P. Lever, Inorganic Electronic spectroscopy, 2nd Ed, Elsevier (1984).
- 12. K. Nakamoto, Infrared and Raman Spectra of Inorganic and Coordination Compounds, 6<sup>th</sup> Ed, Wiley (2009).
- 13. R. B. Jordan, Reaction Mechanisms in Inorganic Chemistry, 2nd Ed, Oxford University Press (1998).
- 14. J. E. Huheey, F. A. Keiter and R.L. Keiter, Inorganic Chemistry: Principles Structure and Reactivity, 4th Ed, Harper Collins (1993).
- 15. J. Burgess, Inorganic Reaction Mechanisms, The Royal Society of Chemistry (1974).

CEM 303: Organic Chemistry General III Marks: 50 Credits: 4 Classes: 70 L

#### Unit-1

## **Stereochemistry-2**

Static and dynamic: conformation and reactivity- cyclic system, Octalines, monocyclic systems-3 to 10 member rings including hetero atom molecules, 6-5, 6-6 including Nitrogenous bicyclic systems, 6-6-6 tricyclic systems. Chiroptical properties of organic molecules: origin, theory; CD, ORD-principles and applications, haloketone rules, sector rules, helicity rules, exceptions and excitation chirality; atomic and conformational asymmetry.

#### Unit-2

## Linear free energy relationship

Hammet equation and its modifications, inductive and resonance effects-σI and σR scales, Taft equation, Yukawa-Tsuno equation, Elucidation of reaction mechanisms, Application of Hammett correlation to heterocyclic systems, Thermodynamic aspects of Hammett equation, Dual substituent parameter (DSP) and Dual substituent parameter-non-linear resonance (DSP-NLR) correlations-Taft-Bromilow-Brownlee approach.

## Unit-3

## Name reactions

Allan–Robinson, Apple, Baylis–Hillman, Borodine-Hunsdiecker, Gombberg-Bachmann, McMurry, Shapiro & Bamford–Stevens, and; Ley, Pfitzner-Moffat, Rubottom and Swern oxidations; Buchwald-Hartwig amination, Corey–Nicolaou macrolactonization, Peterson olefination, Wolff aromatization, Yamaguchi esterification. Mitsunobu reaction, Julia olefination, Click chemistry, Strain promoted azide alkyne cycloaddition (SPAAC) reaction, Staudinger reaction and ligation, Multicomponent reactions (Biginelli reaction, Ugi reaction, Petasis reaction etc.), Prins reaction, Ohira-Bestmann reaction, Bergman cyclization, Wacker oxidation, Grieco oxidation (selenium reagent), Ito oxidation (Pd reagent).

## Unit-4

## **Medicinal chemistry**

Pharmacokinetics: Drug, absorption, distribution, metabolism (Phase-I and Phase-II transformations), excretion, drug formulation.

Pharmacodynamics: drugs and drug targets, drug binding forces, role of enzymes; drug-receptor interactions, mechanism of drug action, agonists, antagonists

Introduction to drug designing

Antibiotics: Penicillins, cephalosporins, macrolides, tetracyclins, etc; new to newer generation of antibiotics Natural Products as Lead Drug: Synthesis and mechanism of anti-tumor, antiviral, anti- sense and DNA cleaving agents.

#### Unit-5

## **Polymer chemistry**

Fundamentals, classification, structure and morphology, different synthetic methods: step-growth, chain-growth mechanism, kinetics of polymerization (condensation, cationic, anionic and radicals); molecular weight and its determination, polydispersity index, thermal transitions, some specific methods for molecular weight determination of biopolymers—gel filtration; SDS—PAGE for proteins, Agarose gel method for nucleic acids; thermodynamics of polymer solution, polymer conformation; polymer engineering. Environmental aspects of polymers.

## **Course Outcomes (CO):**

Upon successful completion of these courses, students will be able to:

Unit 01: Distinguish between static and dynamic stereochemistry, Analyze the relationship between conformation and reactivity, Analyze the conformational preferences of bicyclic and tricyclic systems.

Describe the principles and applications, Apply the haloketone rules, sector rules, and helicity rules to determine the absolute configuration of chiral molecules using CD and ORD data.

Unit 02: Explain the Hammett equation, Apply the Hammett equation to predict the effect of various substituents on reaction rates and equilibrium constants, explain methods for the separation of inductive and resonance effects, physical significance of  $\sigma I$  and  $\sigma R$ . Explain and utilize the Yukawa-Tsuno equation, Extend the application of the Hammett correlation, to elucidate the mechanisms of organic reactions, thermodynamic basis. Understand and apply the Dual Substituent Parameter-Non-Linear Resonance (DSP-NLR) correlations.

Unit 03: Identify, Understand and explain the mechanisms of wide range of important named reactions in organic synthesis, Predict the products of these named reactions.

Unit 04: Explain ADME Processes, Differentiate and explain Metabolic Transformations, Identify Drug Targets, Elucidate Mechanisms of Action of the selected drugs, Define and distinguish between agonists and antagonists, providing examples of their actions

Unit 05: Define basic concepts, classifications, physicochemical properties of polymers, correlate between structure and morphology, Describe and apply average mol wt and PDI, Describe the different types of polymerization mechanism, explain kinetics of condensation, cationic, anionic and radicals, describe methods for determining the molar mass of synthetic as well as biopolymers, Discuss the environmental aspects of polymers.

- 1. J. Hine, Hammett equation C. D. Johnson; Physical Organic Chemistry.
- 2. Peter Sykes, A Guidebook to Mechanism in Organic chemistry.
- 3. W. Caruthers, Modern Methods of Organic Synthesis, 3rd Edn, Cambridge University Press, Cambridge, 1996.
- 4. T. H. Lowry and K. C. Richardson, Mechanism and Theory in Organic Chemistry, 3rd Edn, Harper and Row, New York, 1998.
- 5. H. O. House, Modern Synthetic Reactions, 2nd Edn, Benjamin, 1971.
- 6. P. Deslongchamps, Stereoelectronic Effect in Organic Chemistry, Pergamon Press, Oxford, 1983.
- 7. R. S. Atkinson, Stereoselective Synthesis, Wiley, New York, 1995.
- 8. K. C. Nicolson and E. J. Sorensen, Classics in Total Synthesis, VCH, Weinheim, 1996.
- 9. J. March, Advanced Organic Chemistry: Reactions, Mechanism and Structure, John Wiley, New York, Latest edition.
- 10. F. A. Carey and R. J. Sundberg, Advanced Organic Chemistry, Parts A and B, 4th Edn, Plenum Press, London, 2001.
- 11. J. R. Hanson, Organic Synthetic Methods, Royal Society of Chemistry, London, 2002.
- 12. R. O. C. Norman and J. M. Coxon, Principles of Organic Synthesis, 3rd Edn, ELBS, London, 2003.
- 13. G. L. Patrick, An Introduction to Medicinal Chemistry, 3rd Edn, Oxford University Press Inc, New York, 2005.
- 14. A. Kar, Medicinal Chemistry, 4th Edn, New Age International (P) Ltd, India, 2007.
- 15. C. G. Wermuth, The Practice of Medicinal Chemistry, 3rd Edn, Academic Press, New York, 2008.
- 16. Ashutosh Kar, Medicinal chemistry, 4<sup>th</sup> Edn. New Age International Pub.

- 17. Graham L. Patrick, An Introduction to medicinal chemistry, 3<sup>rd</sup> Edn., Oxford (International student Edn.)
- 18. Medicinal Inorganic chemistry, Edited by J. L. Sessler, S. R. Doctrow, T. J. MeMurry and S. J. Lippard, American chemical society, Washington, DC. (Instant Notes)
- 19. G. Patrick, Medicinal chemistry, Viva Books Pvt. Ltd.
- 20. D. Sriram & P. Yogeeswari, Medicinal chemistry Principles and practice, 2<sup>nd</sup> Edn., Pearson,
- 21. Medicinal Chemistry edited by F. D. King, Royal Society of Chemistry.

## CEM 304: Physical Chemistry General III Marks: 50 Credits:4 Classes:70 L

## Unit-01

## **Spectroscopy-2:**

Raman Spectroscopy: Classical and Q.M theory of Raman scattering, Characteristic parameters of Raman lines, Pure rotation and vibrational Raman spectra; Mutual exclusion principle, Basic principles of a Raman spectrometer, Application of Raman spectroscopy.

Magnetic Resonance Spectroscopy: Introduction to NMR, nuclear spin, chemical shifts, coupling constants and integration; Fourier transform technique; Chemical shifts, coupling constants, Larmor precession, spin-spin and spin-lattice relaxations, Selection rules and relative intensities of lines, Treatment of Chemical Shift and spin-spin coupling in AX, AMX and AB proton NMR, Multi-nuclei NMR, Factors Affection Chemical Shifts; Electron Spin and its Characteristics, Treatment of ESR of hydrogen atom with spin levels, g value and hyperfine interaction in hydrogen atom and free radicals, Mechanism of proton splitting in organic molecules; McConnel Equation; Basic introduction to anisotropic g- and A- tensors from transition ions, Energy levels in many electron spin systems and zero-field splitting.

Mossbauer Spectroscopy: Mossbauer effect and Mossbauer spectroscopy and Mossbauer energy levels with isomer shift, Qudrupole splitting and hyperfine interaction with special reference to Fe57, and Sn119.

## Unit-02

## **Chemical Kinetics-2:**

Kinetics of fast Reaction: Luminescence and energy transfer processes, Study of kinetics by flow and stopped flow techniques, relaxation method, flash photolysis and magnetic resonance method; Theories of unimolecular reactions: Lindemann, Hinshelwood, Rice-Ramsperger-Kassel (RRK) and Rice-Ramsperger-Kassel-Marcus (RRKM) theories, Molecular reaction dynamics-molecular beam experiments, Chemiluminescence.

#### Unit-03

## **Computational Chemistry:**

Introduction to computers in chemistry & Digital literacy: Fundamentals of computers, Introduction to digital literacy: Windows, file management, basic data handling (MS Excel); Overview of computational chemistry and the role of computing in chemical problems.

Basics of computer programming: Elements of computer languages (any one): FORTRAN or C (overview and historical relevance), Constants and variables, Operations and symbols, Expressions and arithmetic assignment statements, Input/Output and format statements, Termination and branching statements (IF, GO TO, LOGICAL variables), Double precision variables.

Applied programming in chemistry: Writing simple programs for: Chemical kinetics equations, Radioactive decay, Solving linear simultaneous equations [Huckel MO theory).

Structural data and visualization tools: Structural features: bond lengths, bond angles using molecular databases (Cambridge Structural Database – CSD) and using ChemOffice and ChemDraw for molecular visualization.

Modern scripting and scientific computing tools: Python programming for: Data manipulation (NumPy, pandas), Plotting (Matplotlib), Automation of tasks; Introduction to Avogadro: Running simple molecular simulations or visualizations.

## Unit-04

#### Colloids and surfaces:

Colloids (kinetic properties, optical phenomena, coagulation), Micelles and reverse micelles, vesicles, microemulsion, Purification and separation of colloids; Electrokinetic phenomena, Osmosis, Dialysis, Gel filtration and Ultracentrifugation; Nano particles: Definition, characteristics classification, synthesis and applications, Quantization of energy states, Structure property relationship of the nanomaterials, Potential applications of nanoscience in chemistry, biology, environment, energy conversion, electronics, magnetic applications; Thermodynamics at the interfaces, Electrostatic and electrokinetic phenomena; BET and other isotherms, Surface energy, defects, steps, kinks, solid-liquids, solid-gas phase reactions; Operando spectroscopy; Surfaces: nanostructures, mesopores and nanopores; Zeolites and clays, Chemical reactivity and selectivity of the nanopore surfaces.

#### Unit-05

## **Electrochemistry: Ions in solution:**

Debye-Huckel theory: its modifications and extensions, mean ionic activity co-efficients, ion association, and precise determination of dissociation constants of weak electrolytes by method of emf and conductance measurements, ion-solvent interaction and solvation number.

Ion-Association: Bjerrum and Fuoss equation for ion-pair formation; Conductance minima, ion-triplet, ion-quadruplets; Walden's empirical rule and Fuoss treatment of conductance minima; Fuoss-Shedlovsky's method of determination of association constant, Ion-transport in solution: Fick laws and equations of Einstein on diffusion; Limiting Debye Huckel-Onsager Expression, Wien Effect, Debye-Falkenhagen effect.

## **Course Outcome (C.O.):**

After the completion of this course, students will be equipped with a deep understanding of advanced spectroscopic, kinetic, thermodynamic, colloidal, and electrochemical principles, blending theories with modern techniques to explore molecular structure, dynamics, and interfacial phenomena.

#### **Reference Books:**

- 1. N. Banwell & E. M. McCash Fundamentals of Molecular Spectroscopy
- **2.** Atkins & de Paula *Physical Chemistry*.
- **3.** P. S. Sindhu *Molecular Spectroscopy*.
- **4.** G. Aruldhas *Molecular Structure and Spectroscopy*.
- **5.** K. J. Laidler *Chemical Kinetics*.
- **6.** D. A. McQuarrie *Statistical Thermodynamics*.
- 7. M. C. Gupta *Statistical Thermodynamic.s*
- **8.** Hiemenz and Rajagopalan *Principles of Colloid and Surface Chemistry*.
- **9.** B. P. Bahadur & G. S. Chatwal *Surface Chemistry and Colloid.s*
- **10.** B. R. Puri, L. R. Sharma, & M. S. Pathania *Principles of Physical Chemistry*.
- **11.** S. Glasstone *An Introduction to Electrochemistry*.
- **12.** J. OM Bockris & A.K.N. Reddy *Modern Electrochemistry V-1,2*.

## CEM 395: Physical Chemistry Practical II Marks: 50 Credits: 4 Classes: 90 L

- 1. Determination of  $pK_1$  and  $pK_2$  of phosphoric acid potentiometrically.
- 2. Determination of CMC and micelization parameters of an ionic surfactant conductometrically.
- 3. Enzyme kinetics.
- 4. Study the effect of ionic strength on the kinetics of  $K_2S_2O_8 + KI$  reaction.
- 5. Study the kinetics of inversion of cane sugar polarimetrically.
- 6. Tensiometric study on the micellization of a non-ionic surfactant.
- 7. Studies on the effect of ionic strength on the micellization of SDS.
- 8. Spectral studies on Py I<sub>2</sub> charge transfer complex.

9. Activity for computational chemistry (any one): (i) Write a simple Python program that builds and solves the Huckel matrix for a linear conjugated system (ii) Hands-on with Avogadro or Chem Draw for running simple molecular simulation and visualization.

Course Outcomes (C.O.):
Reference Books:

CEM 396: Organic Chemistry Practical II Marks: 50 Credits: 4 Classes: 90 L

- (a) Quantitative analysis
- i) Estimation of ascorbic acid by iodometric titration, estimation of ascorbic acid in vitamin C tablet.
- ii) Estimation of number of 1,2-diols by periodic acid oxidation in tartaric acid, glucose and sucrose.
- (b) Multi step organic synthesis (organic solid end product)
- 1) Benzoin to benzyl to benzoic acid to diphenyl acetic acid.

#### **Course Outcomes (C.O.):**

Upon successful completion of these courses, students will be able to Apply iodometric titration to quantitative analysis, Estimate ascorbic acid in both its pure form and in tablet formulations, Apply the chemistry of periodic acid to the quantitative determination of 1,2-diol groups, estimate number of such group in the carbohydrate samples. Design simple synthetic routes, Select appropriate reagents and conditions, Perform practical synthesis including isolation of product in pure form and characterization.

## **Reference Books:**

## **SEMESTER-IV**

CEM 401: Advanced General Marks: 50 Credits: 4 Classes: 70 L

## Unit 01

## **Separation Techniques:**

Successive extraction and separation; techniques of solvent extraction: Craig extraction and counter current distribution; ionic liquid assisted- and supercritical solvent extractions; chromatography: mathematical relationship of capacity, selectivity factor, distribution constant and retention time; chromatogram, elution in column chromatography, band broadening and column efficiency, column resolution; gas liquid chromatography (GLC), van Deemter equation, high performance liquid chromatography (HPLC), thin layer chromatography (TLC), paper chromatography, supercritical fluid chromatography, ion-chromatography, size-exclusion chromatography and capillary electrophoresis: principles, methods, comparison and applications.

#### Unit 02

## **Supramolecular Chemistry**

Concept and language, new horizon and scientific/technological landscape, building blocks: geometry setter, blocker, spacer and counter ions; atomic/ molecular valence, bifunctional ligand, supramolecular orbital, pallet of non-covalent forces like H- bonding,  $\pi...\pi$  interactions; synthesis using secondary building units, modular chemistry and reticular chemistry; supramolecular arrays/- isomerism; isolation of different advanced functional materials; allosterism, principle of three C's, lock and key principle, host-guest interaction, superstructures in inorganic/metallo-organic/ organometallic compounds; innocent OD-/smart 1D-/flat 2D-/intriguing 3D-architectures/hierarchies, supramolecular devices.

## Unit 03 Materials Chemistry

Molecules and crystals to materials, scaffold, art of synthesis, interwoven bonding, molecular aggregates and crystalline architectures; inter-molecular/inter-ion interaction, intercalation materials, dangling bonds, surface functionalization, core-corona in materials science, hysteresis, robust and directional interactions; click chemistry- its characteristics, examples and applications of click reactions; functional materials: conducting, superconducting, magnetic, nonlinear optics, porous, luminous, quantum dots, liquid crystals, liquid crystal display, light emitting diodes, catalysts, molecular and electronic devices, molecular machines, biosensor, biomineralization, proteomics, organic soft materials, proton and hydride sponges, complex electronic oxides, ceramics, composites; materialscharacterization techniques (*viz.*,UV -Vis Spectroscopy, FTIR, Mass Spectrometry, XRD spectroscopy, Scanning Electron Microscopy, Transmission Electron Microscopy, Atomic Force Microscopy, etc.), principles and applications of SEM, TEM, AFM; correlation between materials structures and properties.

## Unit 04 Crystallography

Diffraction of X-ray, Bragg's condition, Bragg's law in reciprocal lattice, Ewald sphere; X-ray crystallography instrumentation, goniometer, geometric data collection, crystal mosaicity and beam divergence, completeness of data collection, crystal to detector distance vs resolution, atomic scattering factor, structure factor, intensity of diffracted beam, Friedel's law, temperature factor on the intensity of diffracted beam, R value and its significance; principles and applications of electron and neutron diffraction methods.

#### Unit 05

## **Green Chemistry**

12- principles, green alternatives for chemical reactions, green catalysts, green solvents, supercritical fluids, green strategies for sample pretreatment, solvent free reaction, ultrasound- and microwave – assisted analytical and synthesis processes, one-pot syntheses, chemicals from renewable feedstocks, green polymers, clean energy - hydrogen fuel; practicing green chemistry in class-room laboratories; sustainable development and green chemistry.

## **Course Outcome (C.O.):**

The learners will have the ability to acquire knowledge for understanding (i) principles of separation using solvent extraction and chromatography, (ii) different methods of extraction and chromatographic systems, (iii) discussions on GLC, HPLC, TLC, paper electrophoresis, size- exclusion chromatography.

The students are expected to understand(i) the basic concepts and principle, molecular recognition and host- guest interactions; (ii) the importance of supramolecular chemistry,(iii) applications in various devices, assemblies and their significance. The learners will have the ability to acquire knowledge for understanding(i) click chemistry, (ii) functional materials, (iii) materials characterization techniques.

The learners are expected to understand (i) fundamentals of X-ray crystallography, crystal classes and their properties, experimental diffraction methods; (ii) methods of growing single crystals, data collection, structure solution, structure refinement and R value, (iii) principles and applications of electron and neutron diffraction methods.

The students are expected to acquire knowledge about (i) green chemistry - set of principles, green methods, sample dissolution, green synthetic methods (ii) use of ionic liquids, supercritical fluids, ultrasonic and microwave radiation, (iii) practicing green chemistry in class-room laboratories.

- 1. D. G. Peters, J.M. Hayes and G.M.Hieftje, Chemical Separations and Measurements, W. B. Saunders
- Company (1974).
- 2. A. Braithinte and F. J. Smitty, Chromatographic Methods, 5th Ed, Springer-Science Business Media, B.V. (1996).
- 3. C. E. Meloan, Chemical Separations: Principles, Techniques and Experiments, 1<sup>st</sup> Ed, Wiley-Interscience (1999).

- 4. J. W. Steed and J. L. Atwood, Supramolecular chemistry, 3rd Ed, Wiley (2022).
- 5. C. Housecroft (Ed.), Supramolecular Chemistry in the 3rd Millennium, MdpiAG(2021).
- 6. J.-M. Lehn, Supramolecular Chemistry: Concepts and Perspectives, Wiley (1995).
- 7. R. Balasubramanian, Callister's Materials Science and Engineering, 2nd Ed, Wiley (2014).
- 8. H. R. Allcock, Introduction to Materials Chemistry, 1st Ed, Wiley (2008).
- 9. Y. Leng, Materials Characterization, 2<sup>nd</sup> Ed, Wiley-VCH (2013).
- 10. A. Haynes, Fundamentals of Crystallography, NY Research Press (2019).
- 11. M. De Graef and M. E. McHenry, Structure of Materials: An Introduction to Crystallography, Diffraction and Symmetry, Cambridge University Press (2012).
- 12. Y. Waseda, X-ray Diffraction Crystallography: Introduction, Examples and Solved Problems, Springer (2011).
- 13. A. K. Das, Elements of Green Chemistry with Green Laboratory Experiments, Readers Service (2014).
- 14. P. T. Anastas and J.C. Warner, Green Chemistry: Theory and Practice, Oxford University Press(2000).
- 15. A. P. Dicks, Green Organic Chemistry in Lecture and Laboratory, 1st Ed, CRC Press (2012).

## CEM -402I: Inorganic Chemistry Special Marks: 50 Credits: 4 Classes: 70 L

## Unit 01

## **Inorganic Chains, Cages and Clusters:**

Polymorphism of C, P and S; inorganic catenation - 1D chain, 2D sheets and 3D networks; homo-/heterocyclic systems; inorganic and coordination polymers, iso- and hetero- chains; homo-/heterocyclic Si-O, P-O rings and cages; low nuclearity and high nuclearity carbonyl clusters, carbide, nitride, chalcogenide and halide containing clusters; M-M bonding (MO approach) in single and multiple bonded compounds, multidecker molecules; Nb, Ta, Mo, W clusters; Zintl, Chini, metalloid, intermetalloid, metallocarborane,water clusters; cluster-surface analogy, structures and bonding, skeletal electron (Elm) counting, Wade-Mingos-Lauher rule; Jemmis' unified mno rules covering PSEPT; applications of metal clusters.

#### Unit 02

## **Bioinorganic Chemistry II:**

Electron transport proteins: cytochromes -cytochrome c, cytochrome c oxidase cytochrome P450 reductase;respiratory electron transport chain, proton pump;chlorophyll and antenna chlorophyll,photosynthetic electron transport chains- PS-I and PS-II, model systems;Mo-enzymes-nitrogenase, sulphite oxidase, nitrate reductase, aldehyde oxidase, xanthine oxidase; nitrogen fixation - biological and abiological; nitric oxide synthase enzyme, vitamin B<sub>12</sub> coenzyme; metal ion interactions with purine and pyrimidine bases, nucleosides, nucleotides and nucleic acids, DNA and RNA.

#### Unit 03

## **Magnetochemistry:**

Basic principles of magnetism, magnetic properties and coordination compounds, spin and orbital moments, spin-orbit coupling, quenching of orbital moment, spin only formula, room temperature and variable temperature magnetic moments; magnetic susceptibility measurements; Curie's law, Curie-Weiss law, Curie-Langevin-Debye equation and their significance; magnetically dilute and concentrated systems, Curie and Neel temperatures, cooperative magnetism, anomalous and subnormal magnetic moments, Bose-Stoner equation, diamagnetic susceptibility, Pascal's constants and its uses; Lande interval rule, microstates, multiplet, multiplet width, hole formalism, energies of J levels, anisotropy in magnetic susceptibility; cryogenic magnetic study, first-/second-order Zeeman effect, van Vleck equation; mechanism of exchange interactions, Bleaney-Bowers equation, Kahn's spin polarization, Goodenough-Kanamori-Anderson rules, antiferro- magnetism, ferromagnetism, spin crossover, spin state isomerism and bistability, single molecule magnet – basic concept, properties and examples.

## **Electrochemical Analysis:**

Introduction to electrochemical methods, electrochemical cells, diffusion controlled limiting current, current- voltage relationship during electrolysis; ion selective electrodes; principles and applicationsof electrogravimetry, coulometry, voltammetry, polarography, differential pulse polarography, anodic stripping voltammetry, amperometry and cyclic voltammetry; Ilkovic equation, Ilkovic- Heyrovsky equation, Nikolskii- Eisenman equation, Cotrell equation, Randles – Sevcic equation and their significance.

#### Unit 05

## **Physical Characterization of Inorganic Compounds-II:**

Mossbauer spectroscopy: Mossbauer effect, nuclear recoil, Doppler effect, instrumentation, chemical shift – examples, quadruple effect, effect of magnetic field, effect of simultaneous electric and magnetic fields, typical spectra of iron and tin compounds; nuclear quadrupole resonance spectroscopy and comparison with Mossbauer spectroscopy.

Electron spin resonance spectroscopy: basic principles, zero field splitting, Kramer's degeneracy, factors affecting 'g' value, isotropic and anisotropic hyperfine coupling constants, spin Hamiltonian, spin densities and McConnell relationship; applications to metal-ligand complexes with paramagnetic metal ions and paramagnetic ligands.

Rotational and vibrational Raman spectroscopy, applications toinorganic diatomic and polyatomic molecules.

## **Course Outcome (C.O.):**

The learners are to (i) appreciate the interesting class of compounds *viz.*, rings, clusters and polymers of metal compounds, (ii) understand structure, bonding, property, reactivity of metal clusters, (iii) explore the wonders of cluster world.

The students will learn aboutmechanism of the action of (i) electron transport proteins, respiratory and photosynthetic electron transport chains, PS-I and PS-II, (ii) Mo-enzymes, biological nitrogen fixation, NOS enzyme and  $B_{12}$ - coenzyme, (iii) metals interaction with DNA, RNA.

The students are to learn (i) magnetic properties and coordination compounds, (ii) magnetic equations, anisotropy in magnetic susceptibility, (iii) mechanism of exchange interactions, spin crossover, spin state isomerism and bistability.

The students know about (i) principles and applications of different electrochemical techniques, (ii)cyclic voltammetry-- its equation and practical aspects, (iii)statement and significance of various electrochemical equations.

The students learn to appreciate basic principles and applications of (i) Mossbauer spectroscopy, (ii) Election Spin Resonance Spectroscopy, (iii) Raman spectroscopy.

- 1. P. Braunstein, L. A. Oro, P. R. Raithby (Eds), Metal Clusters in Chemistry, Wiley-VCH (1999).
- 2. B. Corain, G. Schmid and N. Toshima (Eds), Metal Nanoclusters in Catalysis and Materials Science, Elsevier (2008).
- 3. Z. Luo and S. N. Khanna, Metal Clusters and Their Reactivity. Springer (2020).
- 4. G.N. Mukherjee and A. Das, Elements of Bioinorganic Chemistry, U.N. Dhur & Sons Pvt Ltd (2010).
- 5. S. J. Lippard and J. M. Berg, Principle of Bioinorganic Chemistry, University Science Books (1994).
- 6. D. Ray, Bioinorganic Chemistry, NPTEL Course Material, http://nptel.ac.in/courses/104105031/
- 7. R.L. Carlin, Magnetochemistry, Springer (1986).
- 8. R. L. Dutta and A. Shyamal, Elements of Magnetochemistry, 2<sup>nd</sup> Ed, Affiliated East-West Press (1993).
- 9. N.N. Greenwood and A. Earnshaw, Chemistry of the Elements, 2nd Ed, Butterworth-Heinemann (1997).
- 10. A. J. Bard, L. R. Faulkner and H.S. White, Electrochemical Methods: Fundamentals and Applications, 3rd Ed, Wiley (2022).
- 11. J. O'M. Bockris and AKN Reddy, Modern Electrochemistry, vol 1, 1st Ed, Plenum Press (1970).

- 12. N. Elgrishi, A Practical Guide to Cyclic Voltammetry, SpringerLink (2018).
- 13. V. I. Goldanskii and R.H. Herber (Eds), Applications of Mossbauer Spectroscopy, Academic Press
- 14. R. Das, Principles and Applications of Electron Paramagnetic Resonance Spectroscopy; https://nptel.ac.in/courses/104106048/2
- 15. J. R. Ferraro, K. Nakamoto and C. W. Brown, Introductory Raman Spectroscopy, 2<sup>nd</sup> Ed, Academic Press (2003).

**CEM -402O: Organic Chemistry Special** Marks: 50 Credits: 4 Classes: 70 L

## Unit 01

## **Organometallics**

Applications of Transition metals in Organic synthesis: Organometallic reaction mechanism. Synthetic applications of complexes containing metal-carbon σ-bond: Heck, Kumada, Suzuki, Stille, Sonogashira and Negishi coupling reactions and their applications. Carbon monoxide insertion, Carbon hetero-atom bond formation reactions. Palladium catalysed sequential reactions, Applications of \( \eta\_3\)-allyl palladium and nickel complexes, Synthetic applications of metal alkenes and alkyne complexes: Cobalt-catalyzed reactions (Pauson-Khand and alkyne cyclotrimerization reactions). Applications of metal carbene complexes: Olefin Metathesis reaction and their applications (emphasized on RCM, CM, ROM and eneyne metathesis). Chemistry of arene chromium tricarbonyl complexes, reaction of Fischer and Schrock type carbene complexes, C-H activation.

#### Unit 02

## **Application of Advanced NMR and Mass Spectrometry**

Advanced techniques and applications of NMR: <sup>1</sup>H and <sup>13</sup>C NMR principles, instrumentation, principles of decoupling, gated and inverse gated decoupling, relaxation process, problems on NOE, population transfer. Application of <sup>1</sup>H-<sup>1</sup>HCOSY, <sup>1</sup>H-<sup>13</sup>C HETCOR, HMBC, HMQC, HSQC, NOESY in structure elucidation of organic compounds, solid state <sup>13</sup>C-NMR (CP-MAS) and chemical shift anisotropy.

Advanced mass spectrometric techniques: Realization and application of different ionization techniques: Field ionization, SIMS, FAB, MALDI, ESI, Tandem mass spectrometry and its applications.

## Unit 03

## Carbohydrate chemistry

Synthesis of deoxy- and aminodeoxy sugars; Synthesis of oligosaccharides: Protection & deprotection, glycosyl donor & acceptor and glycosylation reaction, techniques for assembling glycans, Carbohydrate-Chiral pool synthesis (simple molecules), and Carbohydrate based drugs (a few important examples).

#### Unit 04

## Heterocyclic chemistry -2

Fused and extended systems: Purines, pteridines, benzazoles. Six-membered and extended: Pyrimidines, pyridazines, pyrazines

Medium/large rings: Azepines, oxepines, thiepines

Modern Heterocycles: Click chemistry heterocycles (triazoles), Fluorinated heterocycles in pharmaceuticals, Heterocycles in green solvents or ionic liquids

**Applications & Relevance:** Role of key heterocycles in drugs (e.g., omeprazole, sildenafil, allopurinol)

#### Unit 05

#### Supramolecular chemistry

From molecular to supramolecular chemistry: factors leading to strong binding (non-covalent interactions). Molecular receptors: crown ethers: discovery, nomenclature, synthesis, properties and applications; siderophores, cyclophanes, cyclodextrin and their application in specific recognition processes, Supramolecular reactivity and catalysis, Supramolecular sensors, supramolecular aggregates and Nanotechnology.

## **Course Outcomes (C.O.):**

Upon successful completion of these courses, students will be able to:

Unit 01: Discuss and differentiate the mechanisms and synthetic applications of major carbon-carbon bond forming cross-coupling reactions, including Heck, Kumada, Suzuki, Stille, Sonogashira, and Negishi reactions, Explain utility of carbon monoxide insertion and carbon-heteroatom bond formation reactions catalyzed by transition metals, Describe the synthetic applications of metal-alkene and metal-alkyne complexes focusing on Pd and cobalt catalysis, Illustrate metathesis reaction of carbone complexes.

Unit 02: Explain advanced NMR and mass spectrometry techniques to solve the structure of organic molecules and study organic reactions.

Unit 03: explain the significance of deoxy- and aminodeoxy sugars, design synthetic routes for deoxy- and aminodeoxy sugars, identify and apply protecting group strategies for synthesis of glycosyl donor acceptor, explain the mechanism of glycosylation reactions, analyze factors influencing stereoselectivity in glycosylation, design synthetic strategies for oligosaccharides, understand the concept of the carbohydrate-chiral pool, predict reaction outcomes in carbohydrate synthesis.

Unit 04: give systematic name, analyse structure, describe reactivity and design synthesis of the specific heterocycles shown in the content and discuss biological significance and applications.

Unit 05: learn the interactive forces responsible from molecules to supramolecular chemistry, different types of supramolecules along with their formation and applications.

- 1. Ch. Elschenbroich, A. Salzer, Organometallics A concise Introduction.
- 2. Catherine E. Housecroft, Inorganic Chemistry.
- 3. R. H. Crabtree, Organometallic Chemistry of transition Metals.
- 4. B. D. Gupta & A. J. Elias, Basic Organometallic Chemistry.
- 5. C. P. Horwitz& D. F. Shriver, Advances in Organometallic Chemistry, Vol. 23, 1984.
- 6. G. Wilkinson, F. G. A. Stone & E. W. Abel (Eds), Comprehensive Organometallic Chemistry.
- 7. Narendra Pal Singh Chauhan, Narendra Singh Chundawat, Girdhar Pal Singh, Organometallic Reagents in Organic Synthesis.
- 8. Ei-ichi Negishi, Organometallics in Organic Synthesis.
- 9. E. Breitmaier and W.Voelter, 13 C NMR Spectroscopy: Methods and Application in Organic Chemistry, 3rd Edn, Verlag Chemie, 1987.
- 10. M. Duer (Ed), Introduction to Solid State NMR Spectroscopy, Blackwell, 2004.
- 11. T. D. W. Claridge, Tetrahedron Organic Chemistry Series Volume 19, High-Resolution NMR Techniques in Organic Chemistry, Pergamon, Oxford, 2004.
- 12. D. L. Pavia, G. M. Lampman, G. S. Kriz and J. R. Vyvyan, Spectroscopy, Brooks/Cole, a part of Cengage Learning, 2008.
- 13. M. Duer (Ed), Introduction to Solid State NMR Spectroscopy, Blackwell, 2004.
- 14. F. Hillenkamp, J. P. Katalinic, A Practical Guide to MALDI MS: Instrumentation, Method and Applications, 2006.
- 15. H. Budzikiewicz, C. Djerassi and D. H. Williams, Structure Elucidation of Natural Products by Mass Spectrometry, Vol I and Vol II, Holden-Day, 1964.
- 16. N. S. Bhacca, S. Norman and D. H. Williams, Application of NMR Spectroscopy in Organic Chemistry, Holden-Day, 1964.
- 17. H. Budzikiewicz, C. Djerassi and D. H. Williams, Mass Spectrometry of Organic Compounds, Holden Day, 1967.
- 18. R. B. Woodward and R. Hoffman, The Conservation of Orbital Symmetry, Verlag Chemie GmbH, 1970.
- 19. K. Downard, Mass Spectrometry: A Foundation Course, Royal Society of Chemistry, London, 2004.
- 20. C. Dass, An Introduction to Biological Mass Spectrometry, Wiley, New York, 2002.
- 21. G.-J. Boons and K. J. Hale, Organic Synthesis with Carbohydrates.
- 22. The Organic Chemistry of Sugars, Edited by Daniel E. Levy Péter Fügedi.
- 23. P.G.M. Wuts and T.A. Green, Green's protecting groups in organic synthesis.

- 24. Benjamin G. Davis and Antony J. Fairbanks, Carbohydrate Chemistry.
- 25. John A. Joule and Keith Mills, Heterocyclic Chemistry.
- 26. A.R. Katritzky, Comprehensive Heterocyclic Chemistry.
- 27. R. Kartritzky, Handbook of Heterocyclic Chemistry, Pergamon Press, London, 1986.
- 28. P. D. Beer, P.A. Gale and D. K. Smith, Supramolecular Chemistry, Oxford University Press, 1999.
- 29. Supramolecular Chemistry: from Molecules to Nanomaterials, Eds. by P.A. Gale and J.W. Steed (2012).
- 30. F. Diederich, P. J. Stang, R. T. Tykwinski, Modern Supramolecular Chemistry, (2008).
- 31. J. W. Steed, D. R. Turner, K. J. Wallace, Core Concepts in Supramolecular Chemistry and Nanochemistry, (2007).
- 32. J.W. Steed and J.L. Atwood, Supramolecular Chemistry, (2011).
- 33. J.-M. Lehn, Supramolecular Chemistry: Concepts and Perspectives, Wiley VCH, Weinheim (1995).

## CEM -402P: Physical Chemistry Special Marks:50 Credits:4 Classes: 70 L

#### Unit 01

## **Spectroscopy 3**

Time dependent perturbation theory, Harmonic perturbation and transition probabilities, Fermi Golden rule, Induced and spontaneous emission, Einstein transition probabilities, LEASER technique, Vanishing of quantum mechanical integral, Transition probability and symmetry; Application of group theory to molecular vibrations of polyatomic molecules, Normal modes, Vibrational transitions, IR and Raman Spectra and Selection rule, Selection rule for electronic spectra of polyatomic molecules; Principle and application of photoelectron spectroscopy; ESCA and Auger spectroscopy for studies of surfaces.

## Unit 02

## **Photochemistry 2**

Interaction of electromagnetic radiation with molecule: Einstein's treatment on two level transitions; Transition moment integral and its relation with molar extinction coefficient, Basis of selection rule from symmetry argument, Franck Condon principle and its violation, Oscillator strength, Nature of transitions (e.g.,  $n-\pi$ \*,  $\pi-\pi$ \*, d–d, charge transfer etc.), vibronic and spin-orbit coupling; Properties of electronically excited molecules: Redox potential, dipole moment, pK values; Fluorescence life–time; Potential energy diagram for donor acceptor system, Fluorescence anisotropy and its application, Radiative and radiationless processes; Probability and selection rules for radiative transition of absorption, spontaneous and stimulated emission, radiationless transitions; photoinduced energy- and electron-transfer; Examples of quenching experiments by measurements of excited state lifetimes and emission quantum yields: static and dynamic quenching.

## Unit 03

## **Electrochemistry 2**

Electrocatalysis, over potential, exchange current density, Tafel slope, electrode kinetics, reversible, irreversible and quasi-reversible reactions; Structure of electrified interfaces, double layer, zeta-potential; Quantum aspects of charge transfer at the electrode – solution interfaces; Theory and application of polarography and cyclic voltammetry; Corrosion; Photo-electrochemistry; Charge transfer at semiconductor-solution interface; Non-aqueous media: Organic electrolytes, quasi- reference electrode, redox couple, electrochemistry in organic synthesis, electron transfer proton coupled reactions.

#### Unit 04

## **Quantum Chemistry 3**

Degenerate perturbation technique and its application to Stark effect, ground state of hydrogen molecular ion; Introduction to the method of self-consistent Field, Hartree method, Koopman's theorem; Electron spin, Antisymmetry principle, Slater determinant; Many electrons atom, Pure-spin states, Slates-Condon rules, Hartree-Fock theory, Hartree-Fock-Roothaan method; Basis functions, Electron correlation, Configuration interaction; Molecular treatment, Born-Oppenheimer approximation; Valence Bond and

Molecular orbital treatment of Hydrogen Molecule; Introduction to Density Functional Theory.

## Unit 05

## Thermodynamics 3: Irreversible Thermodynamics

Thermodynamic criteria for non-equilibrium process, Entropy production and entropy flow, Entropy balance equations for heat flow, chemical reactions etc., Transformations of the generalized fluxes and forces, Nonequilibrium stationary states, Generalized flux and forces, Phenomenological equations, Onsager reciprocal relations, Principle of detailed balance, Irreversible thermodynamics for biological systems.

## **Course Outcome (C.O.):**

After the completion of this syllabus, students will be empowered with advanced insights into time-dependent quantum mechanics, molecular photochemistry and photophysics, interfacial electrochemistry, many-electron quantum systems, and the thermodynamic principles governing non-equilibrium and biological processes.

#### **Reference Books:**

- **1.** C. N. Banwell & E. M. McCash *Fundamentals of Molecular Spectroscopy*.
- **2.** F. A. Cotton *Chemical Applications of Group Theory.*
- **3.** K. K. Rohatgi-Mukherjee *Fundamentals of Photochemistry*.
- **4.** J. Turro *Modern Molecular Photochemistry*.
- **5.** Bard & Faulkner *Electrochemical Methods: Fundamentals and Applications.*
- **6.** S. Glasstone *An Introduction to Electrochemistry*.
- 7. I. N. Levine *Quantum Chemistry*.
- **8.** S. R. de Groot & P. Mazur *Non-Equilibrium Thermodynamics*.
- **9.** A. Szabo & N. S. Ostlund *Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory.*
- **10.** K. Denbigh *The Principles of Chemical Equilibrium and Non-Equilibrium Thermodynamics*.

## CEM -403I: Inorganic Chemistry Special Marks: 50 Credits: 4 Classes: 70 L

## Unit 01

#### **Nanomaterials:**

Theoretical aspects of 0D, 1D and 2D nanostructures, concept of confinement: quantum dot, quantum wire, quantum wall, quantum transport, control blockade and tunneling condition; effect of quantum confinement on optical properties, optical properties of metallic nanoparticles, core-shell nanoparticles, magnetic properties of nanostructured materials, fullerenes, graphene and carbon materials; synthetic strategies, characterization and applications of nanomaterials.

## Unit 02

## **Inorganic Solid Materials:**

Crystalline solids -- band theory, theories of crystallization and crystal synthesis, methods for growing single crystals, crystal orbital; ionic, covalent, H-bonded, metallic and molecular solids; Laves principles, Zachariasen rules, Ruddlesden- Popper phases, Chevrel phases; silicates - single-/double chain, 3D network, pyroxene, amphibole, talc, mica, clay, zeolite, zeotypes and hyper-/super-tetrahedral frameworks, ZSM-5 and its uses; ferro-/antiferro-/pyro-/piezo- electric materials, solid electrolytes; foreign materials doping, kernel, high entropy alloys and uses; antisite defect, crystallographic shear planes and Wadsley defect.

#### Unit 03

## **Inorganic Photochemistry:**

Photophysical and photochemical processes. excitation modes in transition metal complexes, fate of photoexcited species, fluorescence and phosphorescence applied to inorganic systems, intramolecular energy transfer, vibrational relaxation, internal conversion and intersystem crossing, quantum yield, decay fluorescence; fluorescence quenching, Stern-Volmer equation; examples of different types of inorganic photochemical reactions; photo-substitution and photoelectron transfer reactions in Co, Cr, Ru and Rh complexes, Adamson's rules; photosensitizers, photochemical applications of Ru(bpy)<sub>3</sub><sup>2+</sup> as LAS and LES; photoredox reactions, photocatalysts, photochromism, photochromic coordination complexes; chemical actinometers, chemosensors, fluorescence anisotropy; innersphere and outersphere IT excitations; fluorescence spectrometry and X-ray fluorescence spectrometry -principles, instrumentation and applications in inorganic materials analysis.

#### Unit 04

## **Physical Characterization of Inorganic Compounds-III:**

Atomic spectral methods for trace and ultratrace levels of element analysis; principles, instrumentations and applications of flame photometry, atomic emission spectrometry (AES), atomic absorption spectrometry (AAS) and atomic fluorescence spectrometry (AFS); ideas of flame AAS, electrothermal AAS, cold vapour AAS, hydride generation AAS; inductively coupled plasma (ICP): ICPAES, ICP MS; applications of atomic spectrometric methods in identification and quantification of inorganic species in any matrix.

Thermal methods of analysis; principle and applications of thermogravimetric analysis (TGA), differential thermal analysis (DTA) and differential scanning calorimetry (DSC) for inorganic compounds and solid state reaction kinetics.

#### Unit 05

## Synthetic Methodology for Transition and Non-transition Metal Complexes

Ligand design and ligand syntheses; polypyridine, Schiff base, oxime, macrocycle, tripod, podand, coronand, cryptand, octopus, tailoring and appending of pendant arm, electron reservoir, ligand topology, coordination compound design and synthesis: structure-directed synthesis, metallo-ligand, polymeric ensembles; mechanistic proposal and characterization of the metal complexes.

#### **Course Outcome (C.O.):**

The students are expected to gainknowledge to (i)describe the basic science behind the properties of materials at the nanometer scale, (ii) learn principles of advanced methodologies for studying nanomaterials, (iii) explore synthesis, characterization and applications of nanomaterials.

The learners are expected to have the ability to acquire knowledgewith special reference to (i) theory of crystalline solids and crystallization, (ii) structure and uses of silicates, (iii) foreign materials doping.

The learners are to understand (i) photophysical and photochemical processes, fluorescence and phosphorescence applied to inorganic systems, (ii) photo-substitution and photoelectron transfer reactions, (iii) principle, instrumentation and application of XRF.

The learners are expected to acquire knowledge for understanding (i) atomic spectral processes *viz.*, atomic emission, atomic absorption, atomic fluorescence and ICP atomic emission, (ii) principles and applications of flame photometry, AES, AAS, AFS, ICP-AES and ICP-MS, (iii) thermal methods of analysis using TGA, DTA, DSC.

The learners are expected to (i) study metal/non-metal – ligand complexes synthesis, (ii) gain knowledge of independent thinking in designing and characterizing of transition/non-transition metal complexes, (ii) depict mechanistic proposal of the reactions based on available experimental data.

- 1. T. Pradeep, Textbook of Nanoscience and Nanotechnology, McGraw Hill (2012).
- 2. A. Subramanian and K. Balani, Nanostructure and Nanomaterial: Characteristics and Properties; http://nptel.ac.in/ courses / 118104008
- 3. H. S. Virk (Ed.), Nanomaterials: Basic Concepts and Applications, Scientific.Net (2015).
- 4. L.E. Smart and E. E. Moore, Solid State Chemistry: An Introduction, 3rd Ed, Taylor & Francis (2005).

- 5. H.R. Allcock, Introduction to Materials Chemistry, 1st Ed, Wiley (2008).
- 6. N.N. Greenwood and A. Earnshaw, Chemistry of the Elements, 2nd Ed, Butterworth-Heinemann (1997).
- 7. N. J. Turro, Modern Molecular Photochemistry, University Science Books (1991).
- 8. A. W. Adamson and P.D. Fleischauer, Concepts of Inorganic Photochemistry, Wiley (1975).
- 9. M. Haschke, J. Flock and M. Haller, X- Ray Fluorescence Spectroscopy for Laboratory Applications, Wiley (2021).
- 10. T. R. Dulski, Trace Elemental Analysis of Metals: Methods and Techniques, Routledge (1999).
- 11. A. Fisher, Atomic Spectrometric Methods of Analysis, Royal Society of Chemistry (2025).
- 12. P. J. Haines, Thermal Methods of Analysis: Principles, Applications and Problems, Springer (1995).
- 13. B. D. Gupta, A.J. Elias, Basic Organometallic Chemistry: Concepts, Syntheses and Applications, 2<sup>nd</sup> Ed, Universities Press (2013).
- 14. D. Maiti, Organometallic Chemistry, NPTEL Course Material, IIT Bombay; https://www.youtube.com/watch?v=ITfwjQemwMg&list=PLj\_Alq7xw3018iUgacWidP\_83AOrzqlBR&in dex= 1
- 15. S. Komiya (Ed), Synthesis of Organometallic Compounds: A Practical Guide, Wiley (1997).

CEM -403O: Organic Chemistry Special Marks: 50 Credits: 4 Classes: 70 L

#### Unit 01

## **Asymmetric synthesis**

Syntheses of chiral compounds applying Chiron approach, Advanced Models in Stereoselective Synthesis; Dynamic Kinetic Resolution and Stereodivergence; Curtin–Hammett in the context of asymmetric catalysis, ideas of diastereoselective and enantioselective reactions, basic principles and salient features of asymmetric synthesis; chiral auxiliaries (applications, merits and demerits), asymmetric epoxidation, dihydroxylation and aminohydroxylation, syntheses of commercially and pharmaceutically important chiral compounds using chiral catalysts mainly developed by Knowles, Noyori and Sharpless, asymmetric synthesis of Crixivan (anti-aids compound), asymmetric reduction of unsymmetrical ketones with BINAL-H and CBS reagents, application of chiral oxazaborolidine in the asymmetric Diels-Alder reaction (specially, for the synthesis of the common precursor of prostaglandins), asymmetric C-C bond formation using chiral N-heterocyclic carbene, asymmetric epoxidation of unfunctionalized olefins, principle and applications of asymmetric organocatalysis.

Introduction to Biocatalysis in Asymmetric Synthesis

## Unit 02

## Nucleoside, nucleotide and Nucleic acids

Nucleosides and Nucleotides: structure and nomenclature, chemical synthesis; Hilbert-Johnson reaction, fusion method.

Nuclic Acid: DNA: structure primary (base sequences), and secondary (A, B, and Z forms - brief overview of B-DNA), Chemical Properties: Hydrolysis, modification, Denaturation and renaturation, hybridization, Fundamental Biological Roles: DNA as the carrier of genetic information, replication, transcription - protein biosynthesis.

Structure of RNA, common types of RNA: mRNA, tRNA, rRNA - briefly mention their roles.

## Unit 03

## **Bioorganic chemistry**

Enzymes: Classification, function, enzyme models, kinetics of enzymatic catalysis, serine and cysteine proteases, co-factors, co-enzymes and metalloproteins, Baker's yeast.

Metabolism: Primary and secondary metabolites, their importance and biosynthesis. Carbohydrate metabolism: Glycolysis, TCA-cycle, Glycogen biosynthesis, Glycogenolysis, Reactions of Gluconeogenesis, Cori Cycle, Comparison between Gluconeogenesis and glycolysis Amino acid Metabolism: Oxidative deamination, Transamination, Decarboxylation, Transmethylation, Urea cycle, Fatty acid metabolism: β-oxidation.

#### Unit 04

#### **Reaction intermediates**

Carbenes: Methods of Generation of Carbenes; Reactivity of Carbenes: Addition to Alkenes, Insertion Reactions, Rearrangements and its synthetic applications, Dimerization; Stabilized Carbenes: N-Heterocyclic carbenes (NHCs) - structure, properties, and their role as organocatalysts and ligands in transition metal catalysis.

Nitrenes: Structure, method of generation: Thermolysis and photolysis of azides,  $\alpha$ -elimination from sulphonamides; reactivity: addition to alkenes, insertion reactions: C-H, N-H, and O-H insertion reactions. Selectivity, comparison of carbenes and nitrenes: similarities and differences in their reactivity patterns. Carbene and Nitrene Transfer Reactions using transition metal catalysis.

Radicals in organic synthesis: Basic principles, C-C bond formations by various radical-radical and radical-non-radical coupling reactions. Chain reaction based on stannane chemistry. Syntheses of natural products by using radical reaction as the key steps. Organosamarium and organotitanium reagents. Reduction with iron, copper, ruthenium salts. Dissolving metal reductions. Various ring expansion, ring contraction, remote functionalization and radical fragmentation reaction.

## Unit 05

## Natural products – 2

Derivatized Alkaloids: Structure, transformation and biosynthesis of alkaloids from terrestrial and marine sources; chemistry of quinoline alkaloids with cinchona group, isoquinoline alkaloids with morphine group; alkaloids derived from pyrrolidine, piperidine ring systems and from ring systems containing two N-atoms; peptide alkaloids, macrocyclic alkaloids; chemistry of simple and monoterpenoid derived indole alkaloids – yohimbine, reserpine, strychnine, ellipticine, lysergic acid, representative examples of Iboga and Aspidosperma type indole alkaloids; General study and structural features of sesquiterpenes, diterpenes, triterpenes; chemistry of representative members from the diterpenoid and triterpenoid series.

## **Course Outcomes (C.O.):**

Upon successful completion of these courses, students will be able to:

Unit 01: Understand Foundational Principles of Chirality and Stereoselectivity, Describe and apply the concept of chiron approach, Utilize Chiral Catalysts and Auxiliaries in Asymmetric Synthesis. Analyse Asymmetric Organocatalysis.

Unit 02: Describe and analyse the structure and synthesis of Nucleoside, explain chemical properties of Nucleic acids, explain the structure and role of different RNAs, illustrate replication, transcription - protein biosynthesis.

Unit 03: Describe classifications, different models, and kinetic of catalysis of enzymes. Describe the type and biosynthesis of metabolites. Illustrate the role of cofactor and metabolites. Describe carbohydrate, amino acid and lipid metabolism process.

Unit 04: Define and Classify reactive intermediates, explain Electronic Structure, describe Generation Methods, discuss different factors for reactivity and Stability of radicals, carbenes and nitrenes and their importance in organic synthesis.

Unit 05: Describe structure, transformation, and biosynthesis of different alkaloids from terrestrial and marine sources. Describe structural features and chemistry of sesquiterpenes, diterpenes, triterpenes.

- 1. Robert E. Gawley and Jeffrey Aubé, rinciples of Asymmetric Synthesis.
- **2.** Ernest L. Eliel, Samuel H. Wilen, Lewis N. Mander, Stereochemistry of organic compounds.
- 3. G. Michael Blackburn, Martin Egli, Michael J. Gait, and Jonathan K. Watts, Nucleic Acids in Chemistry and Biology.
- 4. V. Malathi, Molecular Biology.
- 5. U. Satyanarayana and U. Chakrapani, Textbook of Biochemistry.
- 6. Lehninger, Principles of Biochemistry.
- 7. Maya Shankar Singh, Reactive Intermediates in Organic Chemistry.

- 8. Francis A. Carey and Richard J. Sundberg, Advanced Organic Chemistry: Part A: Structure and Mechanisms.
- 9. Giese, Radicals in Organic Synthesis,
- 10. Perkins, Radical chemistry and fundamentals.
- 11. Moody and Whitham, Reactive Intermediates, Oxford University series.
- 12. K. Nakanishi, T Goto, Sho Ito, S. Natori, and S. Nozoe, Natural Products Chemistry, Vol I (1974) and Vol II (1975), Academic Press, New York.
- 13. K. W. Bentley, The Alkaoids, Part II, Interscience Publishers, Wiley, New York, 1965.
- 14. S. W. Pelletier, Chemistry of the Alkaloids, Van Nostrand Reinhold Co, 1970.
- 15. G. F. Cordell, edited, The Alkaloids: Chemistry and Biology, Book series, several volumes.
- 16. P. S. Kalsi, Relevant parts from Natural Products; Vols. I & II.

CEM -403P: Physical Chemistry Special Marks: 50 Credits: 4 Classes: 70 L

#### Unit 01

## **Photophysical processes:**

Photophysical processes of unimolecular processes, Delayed fluorescence, Kinetics of bimolecular processes: collision quenching, Stern-Volmer equation, Concentration dependence of quenching and excimer formation; Excited state electron transfer processes: Exciplex, Twisted intramolecular charge transfer processes, Proton couple electron transfer processes (both intra and intermolecular); Photoinduced electron transfer (PET), intramolecular charge transfer (ICT), twisted intramolecular charge transfer (TICT), electronic energy transfer (EET), and Forster resonance energy transfer (FRET), excited-state intramolecular proton transfer (ESIPT) and aggregation-induced emission (AIE) phenomena extensively along with their detail photophysical properties and application in various filed.

## Unit 02

## **Instrumental Methods of Chemical Analysis:**

Systematic and random errors, Accuracy and precision, regression analysis (least-square method for linear plots), statistics of sampling and detection limit evaluation; Electrochromatography: principle and applications; Thermal analysis: general principles of thermal analysis, Thermogravimetric analysis (TGA): principles, instrumentation, thermogram study, applications, limitations, differential thermogram (DTG); Differential scanning calorimetry (DSC): principles, instrumentation, thermogram study, applications and limitations; Basic principles of electron microscopy—scanning electron microscopy (SEM) and transmission electron microscopy (TEM): instrumentation, sample preparation, applications and limitations; Principle, Instrumentation and application of UV-Vis-NIR spectroscopy, IR spectroscopy, Raman spectroscopy, Fluorescence spectroscopy, Mössbauer spectroscopy, Atomic absorption spectroscopy, ESR, X-ray crystallography, Redox chemistry and Spectro-electro chemistry, NMR spectroscopy, Mass spectrometry, GC and HPLC.

## Unit 03

## **Advanced Materials:**

Introduction to nanomaterials, Physics of low-dimensional materials, 1D, 2D and 3D confinement, Density of states, Excitons, Quantum confinement effect, Zero-, One-, Two- and Three- dimensional structure, Synthesis approach (Top down and bottom up), physical and chemical techniques for nanomaterial synthesis, Size control of metal nanomaterials and their properties: optical, electronic, magnetic properties; surface plasmon resonance, change of bandgap; metal nanoparticles (Au, Ag and Cu), quantum dots, carbon nanotube, graphene, perovskites, nanoclusters, nano-aggregates, micelles, vesicles and worm-like micelles; Supramolecular-assembled structures; Characterizations of nanomaterials with X-Ray Diffraction, Scanning Electron Microscopy, Transmission Electron Microscopy, UV-vis and Photoluminescence; Application of nanomaterials: biomedical usages (drug delivery, cancer treatment, imaging and diagnosis), catalysis, solar cells, energy conversion processes (water splitting), light emitting devices (LEDs), optical sensors, actuators, optical switches, bio-MEMS diodes and nano-wire transistors - data memory lighting and displays, filters, water purification and environmental clean-up, Future scope of

Nanomaterials.

## Unit 04

## **Statistical Thermodynamics:**

Concept of distribution, thermodynamic probability and most probable distribution, Ensemble averaging, Postulates of ensemble averaging, Canonical, grand canonical and micro canonical ensembles, corresponding distribution laws (using Lagrange's method of undermined multipliers); Thermodynamic probability and entropy: Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac statistics, Partition functions-translational, rotational vibrational and electronic partition functions, Calculation of thermodynamic properties in terms of partition functions. Applications of partition functions, Heat capacity behaviour of solids-chemical equilibria and equilibrium constant in terms of partition functions.

#### Unit 05

## **Biophysical Chemistry:**

Hydrophobic effect and self organizing systems, Structure and functions of proteins and nucleic acids and their stability; Structure and functions of cell membranes, Ion transport through cell membrane and nerve conduction; Multiple equilibria; Stacking and co-operative interactions in biological systems; Muscle contraction, Techniques for study of structure & function of proteins and nucleic acids; Structure and function of cell membranes; Ion transport through cell membrane and nerve condition; Introduction to organic drug molecules for biomedical applications; Chemical structure, synthesis and property of important biologically active organic molecules, Biocompatibility, Application of organic molecules in drug delivery, curing human diseases (cancer treatment), Anticancer agents, tissue regeneration, growth and repair, impact of drug smart molecules discovery and development.

**Learning Outcome:** On completion, this syllabus equips students with cutting-edge knowledge in photophysical phenomena, advanced instrumentation, nanomaterials, computational tools, and biophysical chemistry—empowering innovation in molecular diagnostics, materials design, and biomedical science.

#### **References Books:**

- **1.** J. Turro, V. Ramamurthy & J. C. Scaiano *Modern Molecular Photochemistry of Organic Molecule*.
- **2.** K. K. Rohatgi-Mukherjee *Fundamentals of Photochemistry*.
- **3.** G. D. Christian *Analytical Chemistry*.
- **4.** Bard & Faulkner *Electrochemical Methods*.
- **5.** C. N. R. Rao, A. Müller & A. K. Cheetham *The Chemistry of Nanomaterials*.
- **6.** T. Pradeep A Textbook of Nanoscience and Nanotechnology.
- **7.** B. D. Cullity *Elements of X-ray Diffraction*.
- **8.** C. Giacovazzo Fundamentals of Crystallography.
- **9.** Upadhyay, Upadhyay & Nath *Biophysical Chemistry: Principles and Techniques*.
- **10.** C. R. Cantor & P. R. Schimmel *Biophysical Chemistry* (Vol. I–III).

CEM-404: Grand Viva (Marks: 50 Credits: 4 Classes: L)

## CEM – 495: Project (Inorganic/ Organic/ Physical) (Marks: 50 Credits: 4 Classes: L)

Each student has to undertake a Project under the supervision of a faculty member, submit a Project Dissertation and present a seminar on his/her project work. Project works have to be selected on prior consultation of the faculty members of the Department of Chemistry, RRGU. They will be trained in searching research literature, experimental work and computational works as required.

CEM – 496: Internship (Marks: 50 Credits: 4 Classes: L)