Integrated
MSc Chemistry

Faculty of Physical Sciences

(Revised with effect from AY 2022–23 onwards)

Curriculum 5-yr Integrated M Sc – Chemistry 2022

Course Code	Course Title	L T P	Cr	ES	Course Code	Course Title	L T P	Cr	ES
SEMESTER 1					**SEMESTER 2**				
21ENG101	Communicative English	2 0 2	3		21ENG111	Professional Communication	1 0 2	2	
	Language Paper I	1 0 2	2			Language Paper II	1 0 2	2	
22CHY101	General Chemistry I	3 1 0	4		22CHY111	Inorganic Chemistry I	3 1 0	4	
22CHY102	General Chemistry II	3 1 0	4		21ENV200	Environmental Science and Sustainability	3 0 0	3	
22MAT105	Introduction to Calculus and Matrix Theory	3 1 0	4		22MAT116	Ordinary Differential Equations and Vector Calculus	3 1 0	4	
22PHY103	Mechanics	3 1 0	4		22PHY112	Electricity and Magnetism	3 1 0	4	
22PHY182	Physics Lab. I	0 0 2	1		22CHY182	Inorganic Quantitative Lab. – Volumetric Analysis	0 0 2	1	
22ADM101	Glimpses of Indian Culture	2 0 0	2		22PHY183	Physics Lab. II	0 0 2	1	
					22ADM111	Glimpses of Glorious India	2 0 0	2	
					22AVP103	Mastery Over Mind	1 0 2	2	
	TOTAL		**24**			TOTAL		**25**	
SEMESTER 3					**SEMESTER 4**				
22CHY201	Physical Chemistry I	3 1 0	4		22CHY211	Physical Chemistry II	3 1 0	4	
22CHY202	Organic Chemistry I	3 1 0	4		22CHY212	Inorganic Chemistry II	3 1 0	4	
22CHY203	Methodology, Informatics and Analytical principles	3 1 0	4		22MAT221	Integral Transforms	3 1 0	4	
22MAT200	Introduction to Probability and Statistics	3 1 0	4		22PHY214	Waves and Optics	3 1 0	4	
22PHY203	Basic Electronics	3 1 0	4			Open Elective A*	3 0 0	3	
22CHY281	Inorganic Qualitative Lab	0 0 3	1		22CHY282	Basic Organic Qualitative Lab.	0 0 3	1	
21SSK201	Life Skills I	1 0 2	2		21SSK211	Life Skills II	1 0 2	2	
22ADM201	Strategic Lessons from Mahabharata	1 0 0	1		22ADM211	Leadership from Ramayana	1 0 0	1	
	TOTAL		**24**			TOTAL		**23**	
SEMESTER 5					**SEMESTER 6**				
22CHY301	Physical Chemistry III	3 1 0	4		22CHY311	Basics of Analytical Chemistry	3 1 0	4	
22CHY302	Inorganic Chemistry III	3 1 0	4		22CHY312	Organic Chemistry III	3 1 0	4	
22CHY303	Organic Chemistry II	3 1 0	4		22CHY313	Applied Organic Chemistry	3 1 0	4	
	Elective A	3 0 0	3		22CHY314	Basic Spectroscopic Techniques	3 1 0	4	
22CHY381	Physical Chemistry Lab.-Non instrumental	0 0 3	1			Elective B	3 0 0	3	
22CHY382	Organic Synthesis and Estimation Lab.	0 0 3	1		22CHY383	Inorganic Quantitative Lab. – Gravimetric Analysis	0 0 5	2	
22CHY390	Live-in-Lab.[@] / Open Elective B*	3 0 0	3		22CHY384	Physical Chemistry Lab. – Instrumental	0 0 5	2	
21SSK301	Life Skills III	1 0 2	2			TOTAL		**23**	
	TOTAL		**22**		22CHY399	Project (for Exit-option students)		**6**	
								29	
						TOTAL (for Exit-option students)		**147**	
SEMESTER 7					**SEMESTER 8**				
22CHY501	Advanced Physical Chemistry I (Quantum Chemistry)	3 0 0	3		22CHY511	Advanced Physical Chemistry III (Chemical Thermodynamics and Equilibrium)	3 1 0	4	
22CHY506	Advanced Inorganic Chemistry I	3 1 0	4		22CHY516	Advanced Organic Chemistry II	3 1 0	4	
22CHY507	Advanced Organic Chemistry I	3 0 0	3		22CHY504	Advanced Inorganic Chemistry II (Coordination Chemistry)	3 0 0	3	
22CHY512	Molecular Spectroscopy	3 1 0	4		22CHY517	Advanced Organic Chemistry III	3 0 0	3	
22CHY505	Advanced Physical Chemistry II (Group Theory and its Applications)	3 0 0	3		22CHY515	Organometallic Chemistry	3 0 0	3	
22CHY581	Inorganic Semi-micro Qualitative Analysis Lab.	0 0 5	2		22CHY583	Advanced Physical Chemistry Lab.	0 0 5	2	
22CHY582	Organic Quantitative Analysis Lab.	0 0 5	2		22CHY584	Inorganic Quantitative Analysis Lab.	0 0 5	2	
	TOTAL		**21**			TOTAL		**21**	
SEMESTER 9					**SEMESTER 10**				
22CHY605	Advanced Physical Chemistry IV	3 1 0	4						
22CHY606	Advanced Organic Chemistry IV	3 1 0	4		22CHY699	Dissertation		14	
22CHY603	Advanced Inorganic Chemistry III (Solid State Chemistry and Material Science)	3 0 0	3			TOTAL		**14**	
22CHY604	Advanced Inorganic Chemistry IV (Bioinorganic Chemistry)	3 0 0	3						
	Elective	3 0 0	3						
22CHY681	Organic Qualitative Analysis Lab.	0 0 5	2						
22CHY682	Instrumental and Analytical Methods Lab.	0 0 5	2						
	TOTAL		**21**			**GRAND TOTAL**		**218**	
ELECTIVES									
	Electives A& B					**Electives**			
22CHY331	Batteries and Fuel Cells	3 0 0	3	E	22CHY631	Applied Electrochemistry	3 0 0	3	E
22CHY332	Corrosion Science	3 0 0	3	E	22CHY632	Bioanalytical Chemistry	3 0 0	3	E
22CHY333	Green Chemistry	3 0 0	3	E	22CHY633	Chemistry of Biomolecules	3 0 0	3	E
22CHY334	Industrial Catalysis	3 0 0	3	E	22CHY634	Industrial Chemistry	3 0 0	3	E
22CHY335	Introduction to Food Chemistry	3 0 0	3	E	22CHY635	Industrial Stoichiometry	3 0 0	3	E
22CHY336	Polymer Chemistry	3 0 0	3	E	22CHY636	Material Science and Nanochemistry	3 0 0	3	E
22CHY337	Surface Science and Coating Technology	3 0 0	3	E	22CHY637	Medicinal Chemistry	3 0 0	3	E
22CHY338	Forensic Science	3 0 0	**3**	E	22CHY638	Supramolecular Chemistry	3 0 0	3	E

							22CHY639	Nanomaterials for Biomedical Applications	3 0 0	3	E	
							22CHY640	Industrial Metal Finishing Processes	3 0 0	3	E	
							22CHY641	Biosensors: Fundamentals and Applications	3 0 0	3	E	
							22CHY642	Computational Chemistry	3 0 0	3	E	
							22CHY643	Sustainable Chemical Science	3 0 0	3	E	
							22CHY644	Sustainable techniques in Chemical Sciences	3 0 0	3	E	
LANGUAGES												
		Paper I						**Paper II**				
	21HIN101	Hindi I	2 0 0	2	B		21HIN111	Hindi II	2 0 0	2	B	
	21KAN101	Kannada I	2 0 0	2	B		21KAN111	Kannada II	2 0 0	2	B	
	21MAL101	Malayalam I	2 0 0	2	B		21MAL111	Malayalam II	2 0 0	2	B	
	21SAN101	Sanskrit I	2 0 0	2	B		21SAN111	Sanskrit II	2 0 0	2	B	
	21TAM101	Tamil I	2 0 0	2	B		21TAM111	TAMIL II	2 0 0	2	B	

* **Two Open Elective** courses are to be taken by each student, one each at the **4th and the 5th** semesters, from the list of Open electives offered by the School.

@ Students undertaking and registering for a Live-in-Lab project, can be exempted from registering for an Open Elective course in the fifth semester.

SYLLABUS: 5Y INT. MSC CHEMISTRY (2022)

21ENG101 Communicative English 2 0 2 3

Course outcomes

CO 1 Demonstrate competency in all the four linguistic skills, viz. listening, speaking, reading and writing

CO 2 Apply different styles of communication in professional context

CO 3 Participate in different planned & extempore communicative activities

CO 4 Interpret and discuss facts and information in a given context

CO 5 Develop an appreciation for human values

Unit I

Kinds of sentences, Word Order, usage of preposition, use of adjectives, adverbs for description, Determiners- Agreement (Subject – Verb, Pronoun- Antecedent) collocation

Unit II

Tenses

Reported speech

Active and passive Voice

Phrasal Verbs, Linkers/ Discourse Markers, Question Tags

Unit III

Paragraph writing – Cohesion - Development: definition, comparison, classification, contrast, cause and effect - Essay writing: Descriptive and Narrative

Unit IV

Reading Comprehension – Skimming and scanning- inference and deduction – Reading different kinds of material –Speaking**:** Narration of incidents / stories/ anecdotes- Current News Awareness

Unit V

Nirad C Chaudhuri "Indian Crowds" **[Non-Detailed]**

Dr S Radhakrishnan "The Shaping of my Character" [**Detailed**]

Charles Lamb" Dream Children" [**Detailed**]

Ruskin Bond "Night Train at Deoli" **[Non-Detailed]**

Rabindranath Tagore "Subha" **[Non-Detailed]**

Agra Gra " And you call me coloured" [**Detailed**]

Alfred Lord Tennyson "Ulysses" [**Detailed**]

2. Core Reading:

1. Ruskin Bond, *Time Stops at Shamli and Other Stories,* Penguin Books India Pvt Ltd, 1989
2. Syamala, V. *Speak English in Four Easy Steps,* Improve English Foundation Trivandrum: 2006
3. Online sources
4. M Nagarajan, T Sashisekaran, S Ramamurthy *Indian Prose for Effective Communication : A Practical Programme for Colleges* Trinity Press (An imprint of Laxmi Publications Pvt. Ltd.

References:

5. Ruskin Bond, *Time Stops at Shamli and Other Stories,* Penguin Books India Pvt Ltd, 1989
6. Martinet, Thomson, *A Practical English Grammar*, IV Ed. OUP, 1986.
7. Murphy, Raymond, *Murphy's English Grammar,* CUP, 2004

Evaluation Pattern:

Weightage- 50:50

Components	Weightage	Total Marks
Mid Term Exam (Internal)	30 marks	Exam -50
Quizzes and Assignments (Internal)	20 marks	Quizzes-10 Assignments/Presentations-10
End Semester Exam (External)	50 marks	Exam-100

22CHY101 General Chemistry I 3 1 0 4

Course Outcomes

CO1: To understand the various atomic structures based on accepted atom models.
CO2: Predict chemical bonding and molecular geometry based on the existing theories.
CO3: Develop analytical skills for performing volumetric and gravimetric analysis of given samples.

Evaluation Pattern:

Assessment	Internal	External
Periodical 1 (P1)	15	
Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	
End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1 Atomic Structure I

Dalton's atomic theory and its failure, Thomson's experiment charge on electron - Millikan's Oil Drop Technique, e/m ratio of an electron - Chadwick's experiment atomic number, Rutherford's model and its limitations - Maxwell's electromagnetic theory of radiation and his model, Bohr's model of hydrogen atom - Bohr's theory and Ritz combination principle, spectra – emission and absorption - Hydrogen spectrum, Bohr-Sommerfeld theory.

Unit 2 Atomic Structure II

Planck's quantum theory of radiation, dual character of electrons - de Broglie's equation and experiment- Heisenberg's uncertainty principle - photoelectric effect, Compton, Zeeman and Stark effects, Schrodinger wave equation, eigen values, significance of wave function (ψ and ψ^2) and quantum numbers, Schrodinger wave equation for hydrogen and hydrogen-like systems (no derivations, only the final equation), probability distribution of electrons around the nucleus - distribution of 1s, 2s & 2p electrons or orbitals, shapes of atomic orbitals - s, p, d and f, Aufbau principle, Hund's rule, Pauli's exclusion principle, electronic configuration of elements.

Unit 3 Chemical Bonding I

Electrovalency and ionic bond formation, ionic compounds and their properties, lattice energy, Born-Lande

equation and its application, Born-Haber cycle and its application, solvation enthalpy and solubility of ionic compounds, covalent bond, covalency, formation of H_2 in terms of decrease of energy, orbital theory of covalency - sigma and pi bonds - formation of covalent compounds and their properties.

Unit 4 Chemical Bonding II

Hybridization and geometry of covalent molecules - VSEPR theory - polar and non-polar covalent bonds, polarization of covalent bond - polarizing power, polarizability of ions and Fajan's rule, dipole moment, percentage ionic character from dipole moment, dipole moment and structure of molecules, co-ordinate covalent compounds and their characteristics, metallic bond - free electron, valence bond and band theories, weak chemical bonds – inter and intra molecular hydrogen bond - van der Waals forces.

Unit 5 Chemical Analysis and Stoichiometric Calculation

Titrimetry - Fundamental concepts – Theory behind acid base, redox, precipitation and complexometric titrations – problems based on stoichiometry - gravimetry principle and model calculations involving estimation of barium, calcium and nickel - data analysis, significant figures, precision and accuracy – types of errors - mean and standard deviation.

TEXTBOOKS:

1. *F. A. Cotton, G. Wilkinson and P. L. Gaus, 'Basic Inorganic Chemistry', 5th edition, John Wiley, 1987.*
2. *C. N. R. Rao, 'University General Chemistry', Macmillan, India, 2000.*

REFERENCES:

1. *B. R. Puri, L. R. Sharma, M. S. Pathania, 'Principles of Physical Chemistry', Vishal Publishing Co., 2008*
2. *Manas Chanda, 'Atomic Structure and Chemical Bond', 4th edition, Tata McGraw-Hill, New Delhi, 2000.*
3. *Peter Atkins and Julio de Paula, 'Elements of Physical Chemistry', 5th edition, Oxford University Press. 2009.*

22CHY102 General Chemistry II 3 1 0 4

Course Outcomes:

Upon successful completion of this course, the student will be able to

CO1: understand the fundamentals of nuclear science and its applications

CO2: express a substantial knowledge on the fundamental ideas on the structure and properties of solids and liquids.

CO3: analyse the acidic and basic nature of molecules and understanding the chemistry of non aqueous solvents

CO4: understand the water quality parameters and treatment process for domestic and industrial water

Evaluation Pattern:

Assessment	Internal	External
Periodical 1 (P1)	15	
Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	
End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1 Nuclear Chemistry

Size, structure and stability of the nucleus - n/p ratio, packing fraction, mass defect and binding energy - nuclear fission and fusion, atom bombs - hydrogen bomb – radioactivity, alpha, beta particles and gamma radiation - Soddy-Fajan displacement law, half and average life period - Geiger-Muller Counter and Wilson

Cloud Chamber. Applications of radioactivity - in medicine, agriculture, carbon and fossil dating - isotopes, isobars, isotones, isodiapheres and nuclear isomers - natural and artificial radioactivity, artificial transmutation of elements, induced radioactivity, preparation of transuranic elements, Q values, nuclear coulombic barrier.

Unit 2 Solid State

Crystalline and amorphous solids, isotropy and anisotropy, elements of symmetry in crystal systems, indices - Miller indices, space lattice and unit cell, bravais lattices, the seven crystal systems and their Bravais lattices, X-ray diffraction - Bragg's equation and experimental methods (powder method and rotating crystal technique), types of crystals - molecular, covalent, metallic and ionic crystals - close packing of spheres – hexagonal, cubic and body centered cubic packing, interstices in packing - types of crystals – molecular, covalent, metallic crystals - defects in crystals – stoichiometric, non-stoichiometric, extrinsic and intrinsic defects.

Unit 3 Liquid State

Properties of liquids-viscosity, surface tension, capillary action, evaporation, vapour pressure, boiling point and distillation, heat transfer involving liquids. Introduction to liquid crystals, liquid crystal phases-nematic phases, smectic phases; applications of liquid crystals.

Unit 4 Acids, Bases and Non-aqueous Solvents

Concepts of acids and bases – hard and soft acids and bases - Pearson's concept, HSAB principle and its application - basis for hard and soft - soft interactions - non-aqueous solvents - general characteristics of non-aqueous solvents - melting point, boiling point, latent heat of fusion and vaporization, and dielectric constant - reactions such as complex formation, redox, precipitation and acid base type in non-aqueous solvents like liquid ammonia, liquid SO_2 and liquid HF.

Unit 5 Water Technology and Chemical Aspects of Soil

Soft and hard water – Hardness – units of hardness – alkalinity - dissolved oxygen – water for various types of industries – treatment of water by ion exchange process - boiler feed water – boiler compounds – internal and external conditioning - water for drinking - municipal water treatment – desalination by RO and electro dialysis.

Physical properties of soil - Factors affecting soil pH - Soil pH and nutrient availability - Causes of soil degradation. Acid, alkali and saline soils - diagnosis - remediation of acid and salt affected soils. Soil testing - concept, objectives and basis - soil sampling, collection, processing, despatch of soil and water samples. Soil organic matter - its decomposition and effect on soil fertility

TEXTBOOKS:

1. *Marion Clyde Day Jr, Joel Selbin, Harry H Sisler,* '*Theoretical Inorganic Chemistry'*, LLC, 2012
2. *F. A. Cotton and G. Wilkinson, 'Advanced Inorganic Chemistry', 5th edition, John Wiley and Sons, New York, 1987*
3. *B. R. Puri, L. R. Sharma, Kalia, 'Principles of Inorganic Chemistry', Vishal Publishing Co., 2008*
4. *Daji, A.J. 'A Textbook of Soil Science',* Asia Publishing House, Madras, 1970.

REFERENCES:

1. *H. S. Arnicker, 'Essentials of Nuclear Chemistry', 4th edition, New Age International Publishers, 2005.*
2. *L. V. Azaroff, "Introduction to Solids", Mc Graw Hill, New York, 2009*
3. *B. R. Puri, L. R. Sharma, M. S. Pathania, Principles of Physical Chemistry', Vishal Publishing Co., 2008*
4. *Gurdeep Raj, 'Advanced Inorganic Chemistry', 31st edition, Goel Publishing House, 2008.*

22MAT105 INTRODUCTION TO CALCULUS AND MATRIX THEORY 3 1 0 4

CO1: Understand the elementary functions and concepts of limit, continuity, derivative and integral

CO2: Study techniques of differentiation and use it in optimization problems and curve sketching

CO3: Defining Integral as a sum and review integration techniques

C04: Understand the notion of eigenvalues and eigenvectors, analyze the possibility of diagonalization and hence compute a diagonal matrix, if possible.

CO5: Apply the knowledge of diagonalization to transform the given quadratic form into the principal axes form and analyze the given conic section.

CO6: Understand the advantages of the iterative techniques and apply it to solve the system of equations and finding eigenvectors.

Evaluation Pattern:

Assessment	Internal	External
Periodical 1 (P1)	15	
Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	
End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1

Calculus on a Single variable (Based on Textbook 1) Graphs Functions and their graphs. Shifting and scaling of graphs. Limit and Continuity - Limit of Functions, One sided limits and limits at infinity.

Unit 2

Continuous Functions, Discontinuities. Applications of Derivative - Extreme values of functions, Concavity and Curve Sketching.

Unit 3

Integration - Definite Integrals, Properties of definite integrals. Integration techniques. Fundamental theorem of Calculus. Numerical Methods - Trapezoidal and Simpson's rules. (Sections: 1.3, 1.5, 2.3, 2.4, 2.5, 2.6, 4.1, 4.4, 5.3, 5.4, 8.7)

Unit 4

Matrix Eigen Value problems (Based on Text book 2) Linear Independence and rank of a matrix, Eigen values and Eigen vectors- Definitions and properties.

Unit 5

Some applications of eigenvalue problems, Symmetric, Skew Symmetric and Orthogonal matrices, Eigenbases, Diagonalization, Quadratic forms. (Sections: 8.1-8.4) Numerical Methods - Power Method for Eigen Values and Eigen Vectors. (Sections: 20.8)

TEXTBOOKS:

1. Calculus, G. B. Thomas, Pearson, 2009, Eleventh Edition.
2. Advanced Engineering Mathematics, Erwin Kreyszig, Wiley India, Tenth Edition, 2015.

REFERENCE BOOKS;

1. George Turrell, Mathematics for Chemistry and Physics, Academic Press, 2002.
2. Herbert S. Wilf, Applied Mathematics for Physical Chemistry, 2nd Edition, Prentice Hall, 1998.

22PHY103 MECHANICS 3 1 0 4

CO1: Identifying various motions in 1D, 2D, and 3D utilizing the fundamental principles of vectors.

CO2: To learn about the forces involved in motion and Newton's laws of motion.

CO3: To investigate the concept of work and energy to clarify the energy conservation in collisions.

CO4: To study rotational motion and to identify the relation between variables of linear motion and rotational motion.

CO5: Examining the theoretical notion of ideal and damped harmonic oscillations.

Evaluation Pattern:

Assessment	Internal	External
Periodical 1 (P1)	15	
Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	
End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1 Motion

Motion in 1D; vectors, motion in 2D & 3D, projectile and uniform circular motion; relative motion and relative velocity.

Unit 2 Forces and dynamics

Force, mass, Newton's laws, inertial mass, examples of forces, free body diagram analysis for simple applications; friction and contact forces, drag force and terminal speed, uniform circular motion.

Unit 3 Work, Energy, Collisions

Work, kinetic energy, work-kinetic energy theorem, work done by gravitational and spring forces, power; Work and potential energy, conservative forces, conservation of mechanical energy, potential energy curve; Center of mass, Newton's law for system of particles, linear momentum and its conservation, Impulse forces, collisions - elastic and inelastic collisions in 1D and 2D; systems with variable mass - rockets.

Unit 4 Rotational Motion

Rotational variables, linear and angular variables, rotational kinetic energy, rotational inertia; torque, Newton's law for rotation, work, rolling – combined translation and rotation, angular momentum, Newton's law in angular form, system of particles, conservation of angular momentum.

Unit 5 Oscillatory motion

Small oscillations in physical systems; determination of frequency; simple harmonic motion; damped oscillations, resonance.

TEXTBOOK:

Halliday, Resnick, and Walker, Fundamentals of Physics, 8th Extended Ed., Wiley Indian Reprint, 2008, Chap. 1-12, 15

REFERENCES:

1. Young and Freedman, University Physics, 11th Ed, Dorling Kindersley India, 2006
2. Halliday, Resnick, and Krane, Physics, Vol. 1, 5th Ed., Wiley Indian Reprint, 2007
3. Feynamn, Leighton and Sands, "The Feynman Lectures on Physics", Narosa, 1E, 2008

22PHY182 PHYSICS LAB. I 0 0 2 1

CO1: Develop the ability to impart useful knowledge in real-world situations.

CO2: Learning measurement techniques, innovative instrument usage, and their practical applications.

CO3: Recognize the ideas, methods, and applications of fundamental problems in physics, and compare the outcomes to theoretical calculations.

CO4: To conduct some fundamental tests in optics and mechanics and to verify the outcomes.

Evaluation Pattern:

Assessment	Internal	External
Continuous Assessment (CA)*	80	
End Semester		20
Total	**100**	

List of experiments:

1. Surface Tension – Capillary Rise Method.

2. Coefficient of Viscosity - Stoke's Method.

3. The Torsion Pendulum.

a. Moment of Inertia of the Disc.

b. The Rigidity Modules of the Material of Wire.

4. Young's Modulus – Uniform Bending.

5. Spectrometer – Dispersive Power.

6. Liquid Lens – Refractive index of liquid.

7. Laser - Wave length of Laser beam.

8. Laser - Slit Width of the given slit.

9. Magnetometer – Measurement of magnetic flux.

22ADM101 Foundations of Indian Heritage 2-0-0-2

Course Outcomes

CO1 Helps the students to imbibe values into their inner spirit and put it into real life practice.

CO2 Help the students towards achieving the best through the process of transformation of their inner self

CO3 Provides the students an insight into the vision of optimistic future.

Syllabus

Introduction to Indian Culture

Introduction to Amma's life and Teachings

Symbols of Indian Culture

Science and Technology in Ancient India Education in Ancient India

Goals of Life – Purusharthas

Introduction to Vedanta and Bhagavad Gita Introduction to Yoga

Nature and Indian Culture Values from Indian History

Life and work of Great Seers of India (1)

Text Books / References:

1. The Glory of India (in- house publication)

2. The Mother of Sweet Bliss. (Amma's Life & Teachings)

21ENG111 Professional Communication (1-0-2-2)

Course Outcomes (CO)

CO1 Demonstrate competency in oral and written communication.
CO2 Apply different styles of communication in professional context.
CO3 Participate in different planned & extempore communicative activities.
CO4 Interpret and discuss facts and information in a given context.
CO5 Develop critical and analytical thinking.

Evaluation and Grading

Internal	External

Components	Marks	Book review	Marks
Mid-term exam	**50**	(Presentation-10; PPT-5; Report submission-5) (Individual activity; minimum 15 minutes per student) **No end semester exam*	**20**
Continuous assessment	**30** 1. Test-10 2. Group Discussion/Debate -10 3. Assignment -10		

Unit 1

Vocabulary Building: Prefixes and Suffixes; One-word substitutes, Modal auxiliaries, Error Analysis: Position of Adverbs, Redundancy, misplaced modifiers, dangling modifiers – Reported Speech

Unit 2

Instruction, Suggestion & Recommendation - Sounds of English: Stress, Intonation - Essay writing: Analytical and Argumentative

Unit 3

Circulars, Memos – Business Letters - e - mails

Unit 4

Reports: Trip report, incident report, event report - Situational Dialogue - Group Discussion

Unit 5

Mini Project and Presentation

Reference books:

a. FelixaEskey. Tech Talk, University of Michigan. 2005
b. Michael Swan. Practical English Usage, Oxford University Press. 2005
c. Anderson, Paul. Technical Communication: A Reader Centered Approach,V Edition, Hercourt, 2003.
d. Raymond V. Lesikar and Marie E. Flatley. Basic Business Communication, Tata McGraw Hill Pub. Co. New Delhi. 2005. Tenth Edition.
e. Thampi, G. Balamohan. Meeting the World: Writings on Contemporary Issues. Pearson, 2013.
f. Lynch, Tony. Study Listening. New Delhi: CUP, 2008.
g. Kenneth, Anderson, Tony Lynch, Joan Mac Lean. Study Speaking. New Delhi: CUP, 2008.
h. Marks, Jonathan. English Pronunciation in Use. New Delhi: CUP, 2007.
i. Syamala, V. Effective English Communication for You (Functional Grammar, Oral and Written Communication): Emerald, 2002

22CHY111 Inorganic Chemistry I 3 1 0 4

Course Outcome

CO01- Acquiring a firm foundation in the fundamentals of periodic tables
CO02: Understanding the properties of elements in periodic tables
CO03: Gaining knowledge about the compounds of s-, p-, d-, f- block elements
CO04: Understanding of basic and practical applications in various fields of metals and alloy behavior and manufacturing processes

Evaluation Pattern:

Assessment	Internal	External
Periodical 1 (P1)	15	
Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	
End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1 s-Block Elements

Long form of periodic table and classification based on electronic configuration - periodicity in properties – atomic, ionic, covalent radii – ionization potential, electron affinity – electronegativity - effective nuclear charge and their trends in periodic table. Anomalous behavior of 1st element of a group – diagonal relationship. *s-Block elements:* General characteristics – atomic and ionic radii – ionization energies – electropositive character – reducing properties – hydration of ions – flame coloration – lattice energies – chemical properties – extraction of alkali and alkaline earth metals – uses of alkali and alkaline earth metals – complexes of alkali and alkaline earth metals – compounds of alkali and alkaline earth metals and their applications.

Unit 2 p-Block Elements

General characteristics – metallic and non-metallic character – diagonal relationship – extraction – Lewis acids – back bonding – boron compounds. Catenation – structure of graphite – intercalation compounds – metal carbonyls – carbides – silica, silicates, glass manufacturing – zeolites. Allotropy in P and S. compounds of N and P - hydrazine – hydrazoic acid – hydroxyl amine – phosphazines. anomalous behavior of oxygen, structure of ozone. Hydrides, halides, oxides, oxoacids, persulphuric acids, nitrides of group VI and VII elements. Inter halogen compounds and their structure. Isolation of noble gases – preparation, properties, structure and uses of noble gas compounds.

Unit 3 d-Block Elements

Transition metals – general characteristics – metallic character – oxidation states – size – density – melting and boiling points – ionization energy – colour – magnetic properties – reducing properties – catalytic properties – non stoichiometric compounds – complex formation – alloy formation – difference between first row and other two rows. Chemistry of Zr, Ti, V and Mo compounds.

Unit 4 f-Block Elements

Position in the Periodic Table - General characteristics of lanthanides and actinides - lanthanide contraction and its consequences. Isolation of lanthanides from monazite including the ion exchange resin method. Actinides - occurrence and preparation, comparison with lanthanides. Chemistry of thorium and uranium - important compounds - preparation, properties and uses of uranyl nitrate, uranium hexafluoride, thorium dioxide.

Unit 5 Metallurgy

Occurrence of metals based on standard electrode potential – concentration of ores – calcination, roasting and smelting – reduction using carbon and other reducing agents – electrolytic reduction – hydrometallurgy – Ellingham diagram. Refining of metals – electrolytic refining – oxidative refining – zone refining – Van Arkel method. Extractive metallurgy of Li, Ni, ferrous metallurgy – manufacture of steel by open hearth process. Alloys – composition and uses of German silver, brass, bronze, gunmetal, alnico.

TEXTBOOKS

1. *Puri B R, Sharma L R, Kalia K K, 'Principles of Inorganic Chemistry', 23rd edition, S. Chand & Co, New Delhi, 1993.*
2. *Lee J. D., 'Concise Inorganic Chemistry', Black Well Science, UK. 2006*
3. *Soni P. L., 'Text Book of Inorganic Chemistry', S. Chand & Co, New Delhi, 2006.*

REFERENCES

1. *Madan R. D., Tuli G. D and Malik S. M., 'Selected Topics in Inorganic chemistry', S. Chand & Co, New Delhi, 2006.*
2. *S. F. A. Kettle, 'Physical Inorganic Chemistry', Spectrum, 1996.*
3. *B. E. Dogulas, DH McDaniel's and Alexander, 'Concepts and Models of Inorganic Chemistry', Oxford IBH, 1983.*

22CHY182 Inorganic Quantitative Lab: Volumetric Analysis 0 0 2 1

Course outcomes

CO1: Develop the concept of acidity, basicity, concentration of solutions, usage of indicators.

CO2: To understand different types of titrations like acidimetry, dichrometry, permanganometry..

CO3: To estimate the strength of a given solution based on the availability of a counter solution of known concentration.

CO4: To develop lab skills like pipetting, preparation of solution and its dilution usage of burette, determination of end point using different types of indicators.

Evaluation Pattern:

Assessment	Internal	External
Continuous Assessment (CA)*	80	
End Semester		20
Total	**100**	

Acid - Base Titrations

1. Preparation of standard sodium carbonate solution, and standardization of hydrochloric acid (methyl orange indicator). Estimation of sodium hydroxide in solution using phenolphthalein indicator.
2. Preparation of standard oxalic acid solution and standardization of sodium hydroxide solution. Estimation of sulphuric acid in solution.
3. Estimation of sodium hydroxide and sodium carbonate in a mixture (analysis of commercial caustic soda) by double indicator method.

Redox Titrations

Permanganometry

1. Preparation of standard oxalic acid solution and standardization of potassium permanganate solution. Estimation of ammonium iron(II) sulphate in solution.
2. Preparation of standard oxalic acid solution and standardization of potassium permanganate solution. Estimation of hydrogen peroxide solution.
3. Estimation of calcium.
4. Estimation of ferrous iron.

Dichrometry

1. Estimation of ferrous iron using external and internal indicators.
2. Estimation of ferric iron using external and internal indicators.

Iodimetry and Iodometry

1. Standardization of sodium thiosulphate using potassium iodate, electrolytic copper and potassium dichromate.
2. Estimation of As_2O_3 and arsenite
3. Estimation of copper sulphate.
4. Estimation of iron in the given sample of haematite by dichromate method.
5. Estimation of copper in bronze by iodometric method.
6. Estimation of tin in solder using EDTA.

TEXTBOOKS

1. *A. I. Vogel, 'A text book of Qualitative Analyses', 4th edition, Longmans publications, 1985.*
2. *G. Pass & H. Sutcliffe, 'Practical Inorganic Chemistry', 2nd edition, Chapman & Hill, 1974.*

REFERENCES

1. *G. S. Turpin, 'Practical Inorganic chemistry', MacMillan, 1895.*
2. *G. W. Parshall, 'Inorganic Synthesis', Vol. 15, Tata McGraw-Hill Education, 1974.*

22MAT116 ORDINARY DIFFERENTIAL EQUATIONS AND VECTOR CALCULUS 3 1 0 4

CO1. Ability to distinguish between linear, nonlinear and ordinary differential equations.

CO2 . Students will be able to solve firsrt order Ordinary differential equations using a verity of techniques such as separation of variables, integrating factors and exact equations

CO3. Students will able to solve second order linear homogeneous and nonhomogeneous differential equation, and understand the connection between ODE and systems of linear Equations.

CO4. Students can apply their knowledge of Vector Analysis to solve problems in the natural sciences.

CO5. Students will be able to apply the gradient, divergence, and curl operators to vector fields, and understand their physical interpretations.

CO6. Students will learn how to compute and interpret line integrals, surface integrals, and volume integrals of vector fields, and how to apply these concepts to physical and chemical problems

Evaluation Pattern:

Assessment	Internal	External
Periodical 1 (P1)	15	
Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	
End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1

Ordinary Differential Equations: First Order Differential Equations - Basic concepts, Exact ODEs and Integrating factor, Orthogonal trajectories. (Sections 1.1, 1.4, 1.6)

Unit 2

Second Order Differential Equations - Review of linear homogeneous ODE of second order with constant coefficients. Euler-Cauchy Equations. Solution of second order linear non-homogeneous ODE by method of Undetermined Coefficients and by method of Variation of Parameters. (Sections 2.1, 2.2, 2.5, 2.7, 2.10)

Unit 3

System of ODEs - Homogeneous and Non-homogeneous systems with Constant Coefficients. (Sections 4.1, 4.2, 4.6) Numerical Methods - Euler's methods, Runge-Kutta method. (Sec: 21.1)

Unit 4

Vector Calculus: Vector and Scalar Functions, fields, derivatives, Curves, Tangent and normal vectors, Arc Length, gradient, divergence and curl (Sections: 9.4, 9.5, 9.7, 9.8, 9.9).

Unit 5

Line Integral, Line Integrals Independent of Path, Double integrals, Green's Theorem in the Plane, Surfaces for Surface Integrals, Surface Integrals, Triple Integrals – Gauss Divergence Theorem, Stoke's Theorem. (Sections: 10.1 - 10.7 and 10.9).

TEXTBOOK:

Advanced Engineering Mathematics, Erwin Kreyszig, Wiley India, Tenth Edition, 2015.

REFERENCE BOOKS:

1. George Turrell, Mathematics for Chemistry and Physics, Academic Press, 2002.

2. Robert G. Mortimer, Mathematics for Physical Chemistry, 3rd Edition, Elsevier, 2005.

22PHY112 ELECTRICITY AND MAGNETISM 3 1 0 4

Course Outcomes

At the end of the course, the students can

CO1: Gain knowledge of fundamental laws of electrostatics and apply it to calculate the electric field and electric potential.

CO2: Understand the magnetic forces that act on moving charges and apply it to determine the magnetic field.

CO3: Acquire knowledge of concepts of induction, magnetism in matter and apply them to solve related problems.

CO4: Understand the physics of capacitors, resistance and develop skills to solve various electric circuits.

Evaluation Pattern:

Assessment	Internal	External
Periodical 1 (P1)	15	
Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	
End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1 Electric forces and fields

Electric forces, charges, conservation of charge, superposition of electric forces; electric fields, calculation of electric fields of static discrete and continuous charge distributions; Gauss' law and determination of electric fields of simple symmetric charge distributions.

Unit 2 Electric potential and Capacitors

Electrical potential energy and electric potential of discrete and continuous distributions of charges; calculating electric field from potential; potential energy of system of point charges; capacitors and dielectrics.

Unit 3 Magnetostatics

Force due to magnetic fields, Hall effect, circular and helical orbits, magnetic force on a current carrying wire, torque on a current loop, magnetic dipole moment; calculation of magnetic field from current sources using Biot-Savart's law and Ampere's law; solenoids and toroids.

Unit 4 Changing magnetic fields

Faraday's law, Electromagnetic Induction, Self & mutual inductance; Magnetism in matter and Maxwell's equations.

Unit 5 DC and AC Circuits

Electric current, resistance, resistivity, microscopic view; DC circuits involving resistance and capacitance; AC Circuits, RLC circuits, transformers.

TEXTBOOK:

1. *Halliday, Resnick, and Walker, Fundamentals of Physics, 8th Ed., Wiley Indian Reprint, 2008, Chapters 22-33.*

REFERENCES:

1. Halliday, Resnick, and Krane, Physics, Vol. 1, 5th Ed., Wiley Indian Reprint, 2007

2. Young and Freedman, University Physics, 11th Ed, Dorling Kindersley India, 2006

3. Edward Purcell, Electricity and Magnetism, 2e, Tata-McGraw Hill, 2011.

4. Feynamn, Leighton and Sands, "The Feynman Lectures on Physics", Narosa, 1E, 2008

22PHY183 PHYSICS LAB. II 0 0 2 1

CO1: To establish a theoretical framework for the lecture-introduced notions through experimentation.

CO2: To introduce ideas and methods that are widely used in experimental research that could be directly related to the theoretical principles studied throughout the course.

CO3: To examine and interpret the principles of thermal physics, magnetism, mechanics, optics and electronics.

CO4: To develop their capacity for independent thought and problem-solving through a curriculum that emphasizes research.

Evaluation Pattern:

Assessment	Internal	External
Continuous Assessment (CA)*	80	
End Semester		20
Total	**100**	

List of experiments:
1. Lee's disc – Thermal Conductivity of a bad conductor.
2. Solar cell characteristics.
3. Potentio meter – Comparison of emfs.
4. Conversion of galvanometer to Voltmeter.
5. Field along the axis of a coil.
6. Measurement of Laser beam divergence.
7. Spectrometer - i – d – curve.
8. Newton's rings.
9. Meter bridge - Resistance measurement.
10. Ref. index of a Transport bar.
11. Elective field distribution.

22ADM111 Glimpses of Glorious India 2-0-0-2

Course outcomes

CO1 Helps the students to imbibe values into their inner sprit and put it into real life practice.

CO2 Help the students towards achieving the best through the process of transformation of their inner self.

CO3 Provides the students an insight into the vision of optimistic future.

Syllabus

Bhagavad Gita and Life Management

Historicity of Ramayana and Mahabharata

Overview of Patanjali's Yoga Sutras

Highlights of Indian Mythology

Indian Society: Its Strengths and Weaknesses

Role & Position of Women in Indian Society

Indian Models of Economy, Business and Management

Health and Lifestyle related issues

Conservation of cultural heritage

Life and work of Great Seers of India (2)

Text Books

1. The Glory of India (in- house publication)

2. Sanatana Dharma (A Compilation of Amma's teachings on Indian Culture)

22AVP103 Mastery Over Mind (MAOM) 1-0-2- 2

Course Outcomes

Course Outcome 1: To be able to describe what meditation is and to understand its health benefits (CO1)

Course Outcome 2: To understand the causes of stress and how meditation improves well-being (CO2)

Course Outcome 3: To understand the science of meditation. (CO3)

Course Outcome 4: To learn and practice MA OM meditation in daily life. (CO4)

Course Outcome 5: To understand the application of meditation to improve communication and relationships. (CO5)

Course Outcome 6: To be able to understand the power of meditation in compassion-driven action. (CO6)

Evaluation Pattern

The course outcomes are envisaged as four broad categories of assessment with the overall weight of each component as articulated in the Course Assessment Specification (Table 3).

1. Reflective Journal: 20 %

2. Group Activities: 20 %

3. Class Participation: 40%

4. Written Examination: 20%

Syllabus

Unit 1: Describe Meditation and Understand its Benefits (CO1)

A: Importance of meditation. How does meditation help to overcome obstacles in life

B: Understand how meditation works. Understand how meditation helps in improving physical and mental health. Understand how meditation helps in the development of personality.

Unit 2: Causes of Stress and How Meditation Improves Well-being (CO2)

A: Learn how to prepare for meditation. Understand the aids that can help in effectively practicing meditation. Understand the role of sleep, physical activity, and a balanced diet in supporting meditation.

B: Causes of Stress. The problem of not being relaxed. Effects of stress on health. How meditation helps to relieve stress. Basics of stress management at home and the workplace.

Unit 3: The Science of Meditation (CO3)

A: A preliminary understanding of the Science of meditation. What can modern science tell us about this tradition-based method?

B: How meditation helps humanity according to what we know from scientific research

Unit 4: Improving Communication and Relationships (CO5)

How meditation and mindfulness influence interpersonal communication. The role of meditation in improving relationship quality in the family, at the university and in the workplace.

Unit 5: Meditation and Compassion-driven Action (CO6)

Understand how meditation can help to motivate compassion-driven action.

Practicing MA OM Meditation in Daily Life (CO4)

Guided Meditation Sessions following scripts provided (Level One to Level Five) during meditation sessions.

TEXTBOOKS/ REFERENCES:

1. Allen, Cynthia (2020) The Potential Health Benefits of Meditation

2. Sharma, Hari (2022) Meditation: Process and Effects

3. Mayo Clinic Staff (2022, April 29). Meditation: A Simple, Fast Way to Reduce Stress.

4. Seppala E (2022, June 30th Unexpected Ways Meditation Improves Relationships a Lot. Psychology Today

5. Schindler, S., & Friese, M. (2022). The relation of mindfulness and prosocial behavior: What do we (not) know?. Current Opinion in Psychology, 44, 151-156.

6. Amritam Gamaya (2022). Mata Amritanandamayi Mission Trust.

22CHY201 **Physical Chemistry I** **3 1 0 4**

Course Objective: To impart sound knowledge in basic physical chemistry topics like thermodynamics, gas laws equilibrium with a view to lay strong foundation.

CO1: Understand the fundamental properties, laws governing the state and the liquefaction of gaseous molecules.

CO2: Develop sound knowledge in thermodynamic principles (both theoretical and analytical) to predict the spontaneity of chemical and physical processes and exploring their industrial applications

CO3: Apply the fundamental thermodynamics of chemical equilibrium to improve the efficiency of industrial processes

CO4: Understand the properties of different types of solutions for analytical and industrial applications.

Skill: The students will acquire sound knowledge in the properties of gaseous molecules, chemical thermodynamics, chemical equilibrium and solution systems.

Evaluation Pattern:

Assessment	**Internal**	**External**
Periodical 1 (P1)	15	
Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	
End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1 Kinetic Theory of Gases

Kinetic molecular model of gases – Maxwell distribution of velocities and its use in calculating molecular velocities (average, rms and most probable velocity and average kinetic energy) - collision diameter, mean free path and viscosity of gases including their pressure and temperature dependence – relation between mean free path and coefficient of viscosity – behaviour of real gases – deviation of gases from ideal behaviour – compressibility factor – van der Waal's equation of state - its derivation and application in explaining ideal gas behaviour – virial equation of state – van der Waals equation expressed in virial form and calculation of Boyle temperature – isotherms of real gases and their comparison with van der Waal's isotherms – determination of molecular mass by limiting density method – critical phenomena – critical constants and determination.

Unit 2 First Law of Thermodynamics and Thermochemistry

System and surrounding – isolated, closed and open systems - state of the system - intensive and extensive variables. Thermodynamic processes - reversible and irreversible, isothermal and adiabatic processes - state and path functions - exact and inexact differentials, concept of heat and work. First law of thermodynamics – statement. Relation between C_p and C_v, calculation of w, q, dE and dH for expansion of ideal and real gases under isothermal and adiabatic conditions of reversible and irreversible processes. Thermochemistry - enthalpy change of a reaction and different enthalpy changes - relation between enthalpy of reaction at constant volume (q_v) and at constant pressure(q_p) - temperature dependence of heat of reaction - Kirchhoff's equation – heat of solution and dilution, bond energy and its calculation from thermochemical data - integral and differential heats.

Unit 3 Second and Third Laws of Thermodynamics

Second law of thermodynamics - different statements of the law - Carnot's cycle and efficiency of heat engine - Carnot's theorem - thermodynamic scale of temperature - concept of entropy - definition and physical significance of entropy - entropy as a function of P, V and T - entropy changes during phase changes - entropy of mixing - entropy criterion for spontaneous and equilibrium processes in isolated system - Gibb's free energy (G) and Helmholtz free energy (A) - variation of A and G with P, V and T - Gibb's - Helmholtz equation and its applications - thermodynamic equation of state - Maxwell's relations..

Unit 4 Chemical Equilibria

Law of mass action - equilibrium constant – relation between K_p, K_c and K_x – thermodynamic treatment of the law of mass action – van't Hoff reaction isotherm – temperature dependence of the equilibrium constant – van't Hoff equation – pressure dependence of the equilibrium constant K_p and K_c – factors that change the state of equilibrium - Le-Chatelier's principle and its application to chemical and physical equilibria.

Unit 5 Solutions

Mixture - homogeneous and heterogeneous mixtures, solution, solvent, solute - concentration of a solution, methods for expressing concentration - concept of activity and activity coefficients; completely miscible liquid systems - benzene and toluene. Duhem-Margules equation, azeotropes - HCl – water and ethanol - water systems; partially miscible liquid systems: phenol - water, triethanolamine - water and nicotine - water systems. Lower and upper CSTs - effect of impunities on CST, completely immiscible liquids, Nernst distribution law – derivation. Applications - determination of formula of a complex ($KI + I_2 = KI_3$). Solvent extraction - principle and derivation of a general formula of the amount unextracted; colligative properties - relative lowering of vapour pressure, elevation of boiling point, depression in freezing point and osmotic pressure (quantitative treatment), molecular weights from colligative properties.

TEXTBOOKS:

1. *Gurdeep Raj, 'Advanced Physical Chemistry', 35th edition, Goel Publishing House, 2009.*
2. *Puri, Sharma &Pathania, 'Principles of Physical Chemistry', 42nd edition, Vishal Publishing & Co, 2007.*

REFERENCES:

1. *R. Stephen Berry, Stuart A. Rice & John Ross, 'Physical Chemistry', 2nd edition, Oxford University press, 2000.*
2. *Levin, 'Physical Chemistry', 6th edition, Tata McGraw-Hill Education, 2011.*

22CHY202 Organic Chemistry I 3 1 0 4

CO 1. To know about naming different classes of organic compounds

CO 2. Understand the structure and reactivity of different types of cyclic hydrocarbons

CO 3. Learn different concepts about organic reaction mechanisms

CO 4. Understand the concept of aromaticity and the types of reactions shown by these compounds

CO 5. To study the various types of isomerism shown by organic compounds

Evaluation Pattern:

Assessment	Internal	External
Periodical 1 (P1)	15	
Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	
End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1 Basic Concepts in Organic Chemistry
Classification and Nomenclature of organic compounds. Rules of IUPAC system of nomenclature of common organic compounds: (a) substitutive nomenclature of specific type of compounds – bridged compounds, bridged cyclic systems with more rings, spiro compounds, cyclophanes. (b) Saturated compounds with cited prefix- azo-, nitro-, nitroso compounds, azides, acetals and ketals, crown ethers. (c) Compounds with cited suffix- sulfur acids and derivatives, imides, lactones and lactams, (d) Specific species/compounds- Organometallic compounds, isotopically modified compounds, anions, cations, free radicals.

Unit 2 Cyclic Hydrocarbons Recapitulation of structure, nomenclature, and reactivity of aliphatic open chain compounds. Structure, nomenclature, isomerism in cycloalkanes and cycloalkenes, general methods of preparation. Relative stabilities of cycloalkanes - Baeyer's strain theory (evidences and limitations), Sachse – Mohr theory of strainless rings, orbital picture of angle strain, Coulson and Moffit's concept (3 centre two electron bond), condensed ring compounds - bicyclobutanes, prismane, cubane, decalin, adamantane (basic idea only), large ring compounds - muscone, civetone

Unit 3 Fundamentals of Organic Reaction Mechanisms
Meaning of reaction mechanism, drawing electron movements with arrows - curved arrow notation, half headed arrows and double headed arrows, nature of bond fission – homolysis and heterolysis, type of reagents – electrophiles and nucleophiles, type and sub type of following reactions with definition and at least one example each: addition, substitution, elimination, rearrangement. Reactive intermediates with example – carbocations, carbanions, carbenes, nitrenes and carbon free radicals. Electron displacement effects - inductive, inductomeric, electromeric, mesomeric, resonance, hyperconjugation and steric effect. Aliphatic nucleophilic substitutions, mechanism of SN_1 & SN_2, SNi, SN_2' – effects of structure, substrate, solvent, nucleophile, and leaving groups – stereochemistry – Walden inversion. Elimination reactions- Hoffmann and Saytzeff rules – cis and trans eliminations, mechanisms of E_1 and E_2 reactions, E_1cB, elimination versus substitution. Addition reactions - mechanism of addition of bromine and hydrogen halides to double bonds - Markownikoff's rule and peroxide effect. Reduction and oxidation reactions.

Frontier molecular orbitals and organic reactions: Introduction to HOMO and LUMO, classification of nucleophiles and electrophiles based on frontier orbitals, importance of antibonding orbitals; a brief introduction to pericyclic reactions, orbital symmetry considerations in Diels-Alder and electrocyclic reactions. Basic sigmatropic rearrangement: Claisen, Cope and oxy-Cope.

Unit 4 Aromaticity
Concept of resonance - resonance energy, Heat of hydrogenation and heat of combustion of benzene, mention of c-c bond lengths and orbital picture of benzene. Structure of naphthalene, anthracene, and phenanthrene (MO diagram ad resonance energy). Concept of aromaticity, Huckel rule – application to benzenoid – benzene, naphthalene, non – benzenoid – cyclopropenyl cation, cyclopentadienyl anion, and tropylium cation, antiaromatic, nonaromatic compounds. Reactions - general mechanism of electrophilic substitution, effect of further substitution - ortho, para, meta directing groups, ring activation and

deactivation, electronic interpretation of effect of orientation, reactivity of naphthalene towards electrophilic substitution – nitration and sulphonation, aromatic nucleophilic substitution – bimolecular displacement mechanism – elimination – addition mechanism, reactivity and orientation in aromatic nucleophilic substitution.

Unit 5 Isomerism in Organic Compounds

Structural isomerism - chain, position, functional and metamerism. **Stereoisomerism** – definition- classification into optical and geometrical isomerism. Projection formulae- Fischer, flying wedge, sawhorse and Newman projections**. Optical Isomerism** - notation of optical isomers – D, L notation, Cahn –Ingold –Prelog rules, R and S notations for optical isomers with one and two asymmetric carbon atoms, erythro and threo representations. optical activity, optical and specific rotations, asymmetric centre, centre and axis of chirality, axial and planar chirality and helicity; topicity - homotopic, enantiotopic and diastereotopic atoms, groups and faces (including Pro-R, Pro-S, and Re/Si stereodescriptors); chirotopicity and stereogenicity, enantiomers and diastereomers, prochiral faces, enantio- and diastereotopicity, achiral molecules, meaning of (+) and (-), optical purity (enantiomeric excess), absolute and relative configuration, optical purity, stereochemistry of tartaric acid. Elements of symmetry, racemization - methods of racemization (by substitution and tautomerism). Resolution – methods of resolution (mechanical, seeding, biochemical and conversion to diasteroisomers). Asymmetric synthesis (partial and absolute). Optical activity in compound which does not contain asymmetric carbon atoms – biphenyls, allenes.

Geometrical isomerism - cis–trans, syn-anti- and E-Z nomenclature, geometrical isomerism in maleic and fumaric acids and unsymmetrical ketoximes - methods of distinguishing geometrical isomers - melting point, dipole moment, dehydration, and cyclisation.

Conformational Analysis - introduction of terms, conformers, configurations, dihedral angle, torsional strain, conformational analysis of ethane, n-butane including energy diagrams - conformers of cyclohexane (chair, boat and skew boat) – axial and equatorial bonds, ring flipping showing axial and equatorial interconversions, conformations of methyl cyclohexane.

TEXTBOOKS:

1. *Organic Chemistry,* T. W. Graham Solomons, Craig B. Fryhle, John Wiley & Sons; 10th edition (December, 2009)
2. *M. K Jain and S.C Sharma "Modern organic chemistry" 3rd edition visal Pub company 2016*
3. *Morrison and R. N. Boyd, 'Organic Chemistry', 6th Edition, Prentice Hall, 1992.*
4. *D. Nasipuri 'Stereochemistry of Organic Compounds', 2nd Edition, New Age International (P) Ltd., Publishers, 1994.*

REFERENCES:

1. *Peter Sykes, 'A Guide book to Mechanism in Organic Chemistry', 6th Edition, Pearson Education, 2009.*
2. *P. S. Kalsi' 'Organic Reactions and their Mechanisms'', New Age International Publishers, 2009.*
3. *J. Clayden, N. Greeves, S. Warren and P. Wothers, 'Organic Chemistry', 2nd edition, Oxford University Press, 2012.*
4. *K. S. Tewari and N. K. Vishnoi 'Organic Chemistry', 3rd Edition, Vikas Publishing House, 2005.*

22CHY203 Methodology, Informatics and Analytical Principles 3 1 0 4

CO 1. Understand the methods and tools of science and experimentation in science

CO 2. Introduction of some basic concepts about doing research in chemistry

CO 3. Familiarization with various tools and software used in chemistry

CO 4. Discussion of various analytical techniques and safety measures used in the laboratory

Evaluation Pattern:

Assessment	Internal	External
Periodical 1 (P1)	15	
Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	

End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1 Methods and Tools of Science & Experimentation in Science

Revision of scientific theories and laws. Importance of models, simulations and virtual testing in chemistry - Design of an experiment – experimentation - observation – data collection – types of data – examples - interpretation and deduction – reproducibility and replication - units and dimensions - interconversions of units. Record keeping for documentation of experiments. Use of scientific calculators.

Chemistry in the service of man- drugs, food flavouring agents, sweeteners, cosmetics, soaps and detergents, paints, varnishes textiles, dyes, fertilizers, insecticides, fuels etc – examples in each

Unit 2 Research in Chemistry

Selecting a topic – hypothesis - design of an experiment – observation – data collection – experimentation. Documentation of experiments – nature and types of data – typical example. Interpretation and deduction – necessity of units and dimensions – accuracy and precision, variables, correlation and causality, sampling, use of controls, experimental bias, analysis, results, discussion of results, models., statistical analysis of experimental data using computers, mean, mode, deviation, standard deviation. - plotting graph, preparation of seminar papers, project. using computers - familiarising MS Office. Study of latest Nobel prize topics in chemistry (one in the year of study of S3 course).

Unit 3 Introduction to Cheminformatics

Features of the modern personal computer and peripherals, computer network and internet – operating systems and softwares. Data information and knowledge. Knowledge management – internet as a knowledge repository, creating your cyber presence – open access. – open active publishing models – basic concepts of IPR, copy right and patents – plagiarism – cybercrime. Introduction to use of IT in teaching and learning process – educational softwares – INFLIBNET, NICNET, BRNET, NPTEL, VIRTUAL LABS OF MHRD academic services (elementary level only). Basics of cheminformatics, applications of cheminformatics, storage & retrieval, file formats – MOL, SDF, CML, PDB formats, SYBYL Line Notation, SMILES of simple molecules like methane, benzene, cyclohexane. Structure drawing, spread sheet and chemistry related softwares. Molecular visualization tools. Chemical Databases.

Unit 4 Analytical Principles

Inorganic Qualitative Analysis - Common ion effect - solubility product - precipitation of cations. microscale analysis – advantages quantitative analysis.

Theory of Titration – fundamental concepts – mole, molarity, molality, normality, ppm, ppb – primary and secondary standards – problems. Acid-base, redox, precipitation and complexometric titrations. Theory of indicators - acid-base, redox, adsorption and metallochromic indicators.

Chromatography - classification of methods - elementary study of adsorption chromatography, column and thin layer- partition chromatography-paper- ion exchange and gas chromatographic methods.

Gravimetric Analysis - Mechanism of precipitate formation - factors affecting solubility of precipitates – co-precipitation and post precipitation - effect of digestion - washing, drying and ignition of precipitates.

Unit 5 Synthetic Methodologies & Safety Measures in Laboratory

Synthetic Methodology – condensation – addition with examples – separation and purification techniques – sublimation, filtration – crystallisation and precipitation, different types of distillation, solvent extraction, vacuum drying.

Introduction to Lab Safety-Regulatory Requirements - labels, material safety. Knowledge of hazard warning information and symbols. Explosive compounds, potentially dangerous mixtures- fire hazards (idea about flammable solvents, ignition sources used in laboratories, metal hydrides), emergency procedures in chemical splashes to skin and eyes, burns and electric shock. Reactive inorganic reactants and their toxicity (strong acids, bases, halogens, chromates). Hazards due to chemicals, toxic- solids, liquids, gases, and other harmful substances - carcinogenic substances.

REFERENCES

1. *Alexis Leon & Mathews Leon, Computers Today, Leon Vikas*
2. *Soti Shivendra Chandra, Contemporary Science Teaching, Soti Shivendra Publications, New Delhi*
3. *Alexis & Mathews Leon, Fundamentals and Information Technology. Leon Vikas ISBN 08125907890.*
4. *Ramesh Bangia, 'Learning Computer Fundamentals, Khanna Book Publishers, ISBN 818752252b*
5. *Barbara Wilson, Information Technology, The Basics, Thomas Learning.*
6. *Calvin W Tayler and Frank Barron, Scientific Creativity: Its Recognition and Development,*
7. *Louise Cohen, Lawrence Manion& Keith Morrison A Guide to Teaching Practice.*
8. *Encyclopaedia of Modern Methods of Teaching and Learning, Edited V K Rao*
9. *Radha Mohan Research Methods in Education.*
10. *R T Mishra Teaching of information Technology.*
11. *M Ravikumar, Information Technology for Higher Education.*
12. *Kolasani Sunil Kumar, K Ramakrishna and Digumarti Bhaskara Rao Methods of Teaching Chemistry.*
13. *V. Rajaram, Introduction to Information Technology, Prentice Hall.*
14. *Andrew R. Leach and V.J. Gillet, An Introduction to Chemoinformatics*
15. *http://www.vlab.co.in*
16. *http://nptel.iitm.ac.in/*
17. *A. I. Vogel, "Text book of Quantitative Inorganic Analysis".*
18. *Day & Underwood "Quantitative analysis: laboratory manual"*
19. *Comprehensive Practical organic chemistry by A.H Ahluwalia, Renu Aggarwal, 2000, universities press.*
20. *Hazards in chemical laboratories and guide to safe practices in chemical laboratories published by Royal Society of Chemistry.*
21. *Vogel's text book of practical organic chemistry new edition*
22. *https://www.nobelprize.org*

22MAT200 INTRODUCTION TO PROBABILITY AND STATISTICS 3 1 0 4

CO1: Apply key concepts of probability, including discrete and continuous random variables, probability distributions, conditioning, independence, expectations, and variances.

CO2: Define and explain the different statistical distributions (e.g., Normal, Binomial, Poisson) and the typical phenomena that each distribution often describes.

CO3: Apply the basic rules and theorems in probability including Bayes's theorem and the Central Limit Theorem (CLT).

CO4: Define and demonstrate the concepts of estimation and properties of estimators.

CO5: Apply the concepts of interval estimation and confidence intervals.

CO6: Apply the concepts of hypothesis testing and p-value.

CO7: Apply the method of least squares to estimate the parameters in a regression model.

Evaluation Pattern:

Assessment	**Internal**	**External**
Periodical 1 (P1)	15	
Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	
End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1

Probability Concepts: Review of probability concepts - conditional probability - Bayes theorem. Random Variable and Distributions: Introduction to random variable – discrete and
continuous random variables and its distribution functions – mathematical expectations – moment generating function and characteristic function.

Unit 2

Binomial, Poisson, Geometric, Uniform, Exponential. Normal distribution functions (moment generating function, mean, variance and simple problems) – Chebyshev's theorem.
Correlation and Regression: Scatter diagram, simple correlation and simple regression for data.
Theory of Estimation: Population and sample – sampling distributions – determination of sample size – t, F and Chi-square distributions – theory of estimation – types of estimation - point estimation and properties of point estimator - interval estimation methods based on normal, t, F and chi-square distributions.

Unit 4

Testing of Hypothesis: Central limit theorem, large sample tests for mean, variance and proportions - small sample tests for mean and variances – tests based on Chi-square distribution (tests for independence of attributes and goodness-of-fit).

Unit 5

Analysis of Variance (ANOVA): Introduction - analysis of variance – one-way analysis of variance – two way analysis of variance - Latin square design – Two factor factorial design.

TEXTBOOKS:

1. Douglas C. Montgomery and George C. Runger, Applied Statistics and Probability for Engineers, (2005) John Wiley and Sons Inc.
2. J. Ravichandran, "Probability and Statistics for Engineers", Revised Edition 2012, Wiley India.

REFERENCE BOOKS:

1. Ronald E. Walpole, Raymond H. Myers, Sharon L. Myers and Keying Ye, Probability and Statistics for Engineers and Scientists, 8th Edition, Pearson Education Asia, 2007.
1. Sheldon M Ross, Introduction to Probability and Statistical Inference, 3rd Edition, Academic Press.

22PHY203 BASIC ELECTRONICS 3 1 0 4

CO1: To understand the basic concepts regarding semiconductor p-n junction devices

CO2: To solve different electrical networks based on theorems

CO3: To develop the knowledge regarding the use of transistors and diodes for different scientific and household applications

CO4: To understand the basic concept and working of Field effect Transistors and operational amplifiers.

CO5: To learn about the digital electronics and logic gates

Evaluation Pattern:

Assessment	Internal	External
Periodical 1 (P1)	15	
Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	
End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1

Voltage and current - resistors, voltage dividers, voltage and current sources, Thevenin's the-orem, sinusoidal signals, signal amplitudes and decibels, other signals, logic levels, signal sources.

Unit 2

Conduction in metals, semiconductors and insulators, intrinsic semiconductors, n and p mate-rials, conduction by drift and diffusion, The p-n junction, Fermi level ofpn junction, diode equation, Hall effect, diode characteristics, capacitance of a p-n junction, rectification, recti-fier configurations for power supplies, circuit applications of a diode-as a switch, clipping, clamping, different types of diodes - Zener diodes, LEDs, diode lasers, photodiodes, etc.

Unit 3

Transistors - npn and pnp, transistor characteristics - CB, CE and CC configurations, relation between a, b and g, transistor switch, transistor biasing. Feedback circuits. Transistor action, emitter follower, Transistor applications as amplifier. RC coupled amplifier.

Unit 4

Transistor as an oscillator, FET, JFET, MOSFET, etc. Operational amplifiers; differential am-plifier, inverting and non-inverting amplifiers ers. Op-amp applications-integrator, differentia-tor, adder etc. ICs – examples.

Unit 5

Digital electronics: Digital versus analog, logic gates, truth table, discrete circuits for gates, logic identities, minimization and Karnaugh maps.

TEXTBOOK:

Bernar Grob and Mitchel.E.Schultz, Basic Electronics (9th Edition), Tata Mc.Graw Hill, New

Delhi (2003)

REFERENCES:

1. John D.Ryder, Electronic Fundamentals and Applications, Prentice Hall of India Pvt.Ltd. New

Delhi (1983).

2. Albert Paul Malvino, Digital Computer Electronics Tata McGraw Hill Pub. Co. Ltd New Delhi (1983

3. Horowitz and Hill, The art of Electronics (Cambridge University press)

22CHY281 Inorganic Qualitative Lab 0 0 3 1

CO1: To categorize elements into different groups

CO2: To enable the students to develop chemical analytical skills in inorganic qualitative analysis.

CO3: By the end of the course the students are expected to be able to: • Plan various experiments and carry out qualitative analysis of inorganic chemical species. • Apply chemical tests to identify unknown chemical species.

Evaluation Pattern:

Assessment	**Internal**	**External**
Continuous Assessment (CA)*	80	
End Semester		20
Total	**100**	

I. Qualitative Analysis:

Analysis of mixtures containing two anions (one simple and one interfering) and two cations (of different groups) from the following:

Anions - HCO_3^-, CO_3^{2-}, Cl^-, F^-, Br^-, I^-, NO_3^-, BO_3^{3-}, SO_4^{2-} and PO_4^{3-}

Cations - Pb^{2+} Bi^{3+}, Cd^{2+}, Al^{3+}, Fe^{2+}, Fe^{3+}, Mn^{2+}, Zn^{2+}, Ca^{2+}, Sr^{2+}, Ba^{2+}, Mg^{2+}, K^+, Na^+ and NH_4^+, Cu^{2+}, Mn^{2+}.

Note:

1. Mixtures requiring elimination of phosphate and borate radicals should not be given (avoid cat ions like Ba^{2+}, Sr^{2+}, Ca^{2+} and Mn^{2+} when phosphate and borate are given).
2. Combinations like Cl^- and Br^-, I^- and Cl^- and NO_3^- and Br^- shall be avoided.

3. Salts that yield $SrSO_4$, $BaSO_4$, $CaSO_4$, $PbSO_4$ and $FeSO_4$ on double decomposition shall be avoided.
4. The two cations in the mixture should belong to different groups. However, combinations like Mg^{2+} and NH_4^+, K^+ and NH_4^+ can be given.

II. **Preparations:** *(Any six from the following)*

1. Ferrous ammonium sulphate
2. Tetrammine copper (II) sulphate
3. Potassium trisoxalato chromate
4. Prussian Blue
5. Hexammine Cobalt (II) chloride
6. Nickel dimethyl glyoximate
7. Potassium trisoxalato ferrate (III)
8. Tristhioureacopper (I) sulphate
9. Ferric alum
10. Potash alum
11. Mohr Salt from Kipp's waste.

TEXTBOOKS

1. *A. I. Vogel, 'A text book of Qualitative Analyses', 4th edition, Longmans publications, 1985.*
2. *V. V. Ramanujam, 'Inorganic Semi Micro Qualitative Analysis', 3rd edition, The National Publishing Company, 1974.*

REFERENCES

1. *G. Pass & H. Sutcliffe, 'Practical Inorganic Chemistry', 2nd edition, Chapman & Hill, 1974.*
2. *D. A. Skoog and D. M. West, 'Analytical Chemistry - An Introduction', 4th Edition, CBS Publishing Japan Ltd., 1986.*

22CHY211 Physical Chemistry II 3 1 0 4

Course Objective: To develop sound knowledge in the fundamentals of phase equilibria, electrochemistry and kinetics for industrial and research applications.

Course Outcomes

CO1: Understand concept of phase rule, phase diagrams and its applications

CO2: Apply chemical kinetics for improving the yield of various reactions and understand the applicability of temperature and catalysts for doing the same

CO3: Analyse electrochemical systems quantitatively and thermodynamically for industrial applications

Skills: The students will acquire theoretical and applied level knowledge in electrochemistry, phase equilibrium and kinetics for different industrially relevant applications

Evaluation Pattern:

Assessment	Internal	External
Periodical 1 (P1)	15	
Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	
End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1 Phase Equilibria

Definition of terms: phase, components and degrees of freedom – derivation of Gibbs phase rule - application of phase rule to one component system: water, carbon dioxide and sulphur system – reduced phase rule; two component system: simple eutectic system: Pb-Ag system, Pattinson's process. Thermal analysis and cooling curves, compound formation with congruent melting point: Zn – Mg, and incongruent

melting point: Na – K system. Metal systems forming continuous solid solutions and solid solutions with minimum and maximum melting points.

Unit 2 Chemical Kinetics

Molecularity and order of a reaction, rate law expression and rate constant - first, second, third and zero order reactions, pseudo-first order reactions (pseudo-unimolecular reactions), complex reactions - equilibrium and steady state approximations - mechanism of these reactions - effect of temperature on reaction rates - Arrhenius equation and its derivation, activation energy, characteristics of activated complex. Theories of reaction rates – collision theory – derivation of rate constant of bimolecular gases reaction – failure of collision theory – Lindemann's theory of unimolecular reaction. Theory of absolute reaction rates – derivation of rate for a bimolecular reaction – significance of entropy and free energy of activation.

Unit 3 Catalysis

Catalysis – homogeneous and heterogeneous – homogeneous catalysis – kinetic of acid – base reaction and mechanism - theory of homogeneous and heterogeneous catalysis. Heterogeneous catalysis – adsorption – types – chemical and physical, characteristics of adsorption. Different types of adsorption isotherms – Freundlich and Langmuir - enzyme catalysis, difference between enzyme catalysis and general heterogeneous catalysis, factors affecting the rate of enzyme catalysed reactions.

Unit 4 Electrochemistry I

Electrolysis, Faraday's laws of electrolysis, strong and weak electrolytes specific, equivalent and molar conductance, equivalent conductance at infinite dilution and their measurement - Kohlrausch's law and its applications - calculation of equivalent conductance at infinite dilution for weak electrolytes, degree of dissociation of weak electrolytes - solubility of sparingly soluble salts - applications of conductivity measurement - conductometric titrations - acid-base precipitation and complexometric titrations, Ostwald's dilution law and its limitations, common ion effect and its application, concept of pH, indicators, theories of indicators – buffers and their pH - Henderson equation, hydrolysis and example of hydrolysis - relation between K_h, K_b and K_w, transport number (Hittorf number) and its experimental determination - Hittorf's method and moving boundary method.

Unit 5 Electrochemistry II

Potential and its origin – electrical double layer and equilibrium – single electrode potential, standard hydrogen electrode - EMF series and its significance – galvanic cells, IUPAC notation - reversible and irreversible cells, electrodes, calomel and Ag/AgCl reference electrodes - indicator and ion selective (pungor) electrodes and their applications, computation of cell EMF, calculation of thermodynamic quantities of cell reactions (ΔG, ΔH and K). Concentration cells – variation of potential with concentration, Nernst equation and its applications, potentiometric titrations - acid-base, redox and precipitation titrations. Corrosion – basic concept - electrochemical corrosion and its mechanism - cathodic and anodic protection – inhibitors.

TEXTBOOKS

1. *Puri, Sharma & Pathania, 'Principles of Physical Chemistry', 42nd edition, Vishal Publishing Co, 2007.*
2. *Gurdeep Raj, 'Advanced Physical Chemistry', 35th edition, Goel Publishing House, 2009.*

REFERENCES

1. *Glasstone and Lewis, 'Elements of Physical Chemistry', 2nd edition, Macmillan, 1982.*
2. *P. C. Rakshit, 'Physical Chemistry', 7th edition, Sarat Book House, 2001.*
3. *R. Stephen Berry, Stuart A. Rice & John Ross, 'Physical Chemistry', 2nd edition, Oxford University press, 2000.*

22CHY212 Inorganic Chemistry II 3 1 0 4

Course Objective: To provide comprehensive knowledge in synthesis, spectral and magnetic properties. Apply this gained knowledge to industrial inorganic processes and biological sciences.

Course Outcomes

CO1: Understanding the salient features of coordination compounds, to explain coordination number, oxidation state of metal, electronic configuration, nomenclature, ligands, structure and bonding.

CO2: Acquiring the knowledge of spectral and magnetic properties of complexes through CFT and MOT.

CO3: Gaining knowledge on the stability of metal complexes, calculation of thermodynamic parameters, with the help of that complex reactivity can be explained.

CO4: Understanding the bonding of organometallic compounds and its industrial applications.
CO5: Imparting the basic knowledge of catalytic cycle of organometallic compounds ,bio-inorganic elements and metal toxicity.

Skill: The students will acquire basic knowledge in coordination compounds, its spectral and magnetic properties, isomerism, bio-inorganic elements and organometallic compounds.

Evaluation Pattern:

Assessment	Internal	External
Periodical 1 (P1)	15	
Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	
End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1 Coordination Chemistry I

Werner's theory – electronic interpretation of co-ordination compounds - EAN rule – types of ligands – nomenclature, isomerism – stability of complexes – factors influencing stability – application of coordination compounds in qualitative and quantitative analysis. Theories of bonding in coordination compounds – VBT, CFT and MOT. VBT – merits and demerits – CFT – crystal field splitting in tetrahedral and octahedral complexes – factors affecting crystal field splitting – CFSE of complexes – spectrochemical series – explanation of geometry, magnetism and colour on the basis of the above theories.

Unit 2 Coordination Chemistry II

Spectral and magnetic properties of metal complexes - electronic absorption spectrum of $[Ti\ H_2O)_6]^{3+}$ ion. Types of magnetic behavior, spin-only formula, calculation of magnetic moments. Reactivity of metal complexes - labile and inert complexes, ligand substitution reactions – SN_1 and SN_2 substitution reactions of square planar complexes – trans effect and applications of trans effect.

Unit 3 Organometallic Compounds

Definition, classification and nomenclature of organometallic compounds, ylides, classification on the basis of hapticity. Catalytic properties of organometallic compounds - alkene hydrogenation, synthesis of water gas – shift reaction, Zeigler-Natta polymerisation, Wilkinson catalyst - 18 electron rule, metal-alkene complexes, metal-alkyne complexes, carbene and carbyne complexes. Metal nitrosyls and dinitrogen complexes. Metallocenes – ferrocene (preparation and structure only). Dibenzene chromium. Zeise's salt – preparation, properties and structure.

Unit 4 Metal Carbonyls and Metal Clusters

Preparation and properties of mononuclear carbonyls. Structures of $Mo\ (CO)_6$, $Fe\ (CO)_5$ and $Ni(CO)_4$. Polynuclear carbonyls, bridged carbonyls and bonding in metal carbonyls. Preparation and properties of carbonyls of Fe and Ni. Metal clusters - carbonyl and halide clusters, low nuclearity carbonyl clusters and high nuclearity carbonyl clusters, electron counting schemes for $Rh_6(CO)_{16}$ and $[Os_6(CO)_{18}]^{2-}$ metal only clusters (Zintl ions).

Unit 5 Bioinorganic Chemistry

Essential and trace elements in biological systems, myoglobin and haemoglobin, role of myoglobin and haemoglobin in biological systems, mechanism of oxygen transport, cooperativity, Bohr effect. Vitamin B_{12} (structure not expected). Metalloenzymes of zinc, inhibition and poisoning of enzymes. Electron carriers – cytochromes. Role of alkali and alkaline earth metals in biological systems, photosynthesis, Na/K pump. Biological function and toxicity of metals – Fe, Cu, Zn, Cr, Mn, Ni, Co, Cd, Hg and Pb, treatment of metal toxicity. Anti-cancer drugs – cisplatin and carboplatin.

TEXTBOOKS

1. *Puri B R, Sharma L R, Kalia K K, 'Principles of Inorganic Chemistry', 23rd edition, Shoban Lal Nagin Chand & Co, New Delhi, 1993.*
2. *Lee J. D., 'Concise Inorganic Chemistry', Black Well Science, UK. 2006*
3. *Soni P. L., 'Text Book of Inorganic Chemistry', S, Chand & Co, New Delhi, 2006.*

REFERENCES

1. *J.E. Huheey, R.A. Keiter, R.L. Keiter, 'Inorganic Chemistry-Principles of Structure and Reactivity', 4th Edn., Prentice Hall, 1997.*
2. *F. A. Cotton, G. Wilkinson, C. A. Murillo & M. Bochmann, 'Advanced Inorganic Chemistry', 6th edition, John Wiley, 1999.*

22MAT221 INTEGRAL TRANSFORMS 3 1 0 4

CO 1: To enable the students to study the Laplace Transforms, properties of Laplace Transform, inverse Laplace Transform and some applications to solve the differential equations and integral equations.

CO 2: Find the Laplace transform of derivatives, integrals and periodic functions. Use the Method of Laplace transforms to solve initial-value problems for linear differential equations with constant coefficients and system of linear differential equations.

CO 3: Able to understand the Fourier Series, it to find the Fourier series expansion of given functions and to find half range expansions.

CO 4: To enable the students to study Fourier Transforms and some concepts of Fourier Sine and Cosine transforms.

CO 5: Introduce students to partial differential equations and to solve linear Partial Differential with different methods. Also, to derive heat and wave equations in 2D and 3D.

Evaluation Pattern:

Assessment	**Internal**	**External**
Periodical 1 (P1)	15	
Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	
End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1

Laplace Transform: Laplace Transforms, Inverse Transforms, Linearity, Shifting, Transforms of Derivatives and Integrals, Differential Equations, Unit Step Function, Second Shifting Theorem, Dirac's Delta Function.

Unit 2

Differentiation and Integration of Transforms. Convolution, Integral Equations, Partial Frac-tions, Differential Equations, Systems of Differential Equations. (Sections: 6.1 to 6.7)

Unit 3

Fourier Series and Fourier Transform: Fourier series, Half range Expansions, Parseval's Iden-tity, Fourier Integrals, Fourier integral theorem. Sine and Cosine Integrals.

Unit 4

Fourier Transforms, Sine and Cosine Transforms, Properties, Convolution theorem. (Text book-1, Sections: 11.1-11.3, 11.7-11.9)

Unit 5

Applications of Partial Differential Equations: Basic Concepts, Modeling; VibratingString, Wave Equation, Separation of Variables, Use of Fourier Series, Heat Equation; Solution by Fourier Series. (Sections: 12.1, 12.2, 12.3, 12.4)

TEXTBOOK:

1. Advanced Engineering Mathematics, E Kreyszig, John Wiley and Sons, Tenth Edition, 2015.

REFERENCE BOOKS:

1. George Turrell, Mathematics for Chemistry and Physics, Academic Press, 2002.

2. Donald Allan McQuarrie, Mathematics for Physical Chemistry, University Science books, 2008.

22PHY214 WAVES AND OPTICS 3 1 0 4

CO1: Reviewing the basic concepts of geometrical optics

CO2: To examine the various forms of oscillation and relate the concept to that of waves.

CO3: To conceptually understand the interference phenomena and to learn its various manifestations.

CO4: To evaluate different diffraction phenomena scenarios, as well as to study the production and analysis of polarized light.

CO5: Investigate the applications of optics in field of optical fibers and holography.

Evaluation Pattern:

Assessment	**Internal**	**External**
Periodical 1 (P1)	15	
Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	
End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1

Review of Geometrical Optics: Fermat's principle, laws of reflection and refraction from Fermat's principle. Refraction at a spherical surface, Linear and lateral magnifications, Refraction through a thick lens. Focal lengths of thick and thin lenses. Combination of two lenses. Cardinal points.

Unit 2

Wavemotion: Simple Harmonic Oscillation (SHO), differential equation for SHO and its general solution, super position of two or more SHOs, Damped and forced oscillators, resonance. Wave equation, travelling and standing waves in one dimension, energy density and energy transmission in waves, Group velocity and phase velocity.

Unit 3

Interference: Wave nature of light, Spatial and temporal coherence, coherent sources, interference of light by division of wave front: Fresnel's biprism, interference of light by division of amplitude: interference in thin films, fringes of equal inclination, airwedge, Newton's rings and Michelson's interferometer. Multiple beam Interference -

Fabry-Perot interferometer, multilayer thinfilms: AR and HR coatings.Diffraction: Fresnel and fraunhoffer diffraction, diffraction grating, Rayleigh criterionand resolving power.

Polarisation: linear, circular and Elliptic polarization, double refraction and optical rotation. Propagation of light through matter, dispersion and absorption, Nonlinear optics, second harmonic generation, integrated optics (qualitative only).

Unit 5

Fiber optics: Introduction to optical fiber, the numerical aperture, coherent bundle, pulse dispersion in step index fiber, graded index fiber, single mode fiber, multimode fiber, fiber optic sensors - examples - fiber optic communication (qualitative), Advantages of fiber optic communication system.

REFERENCES:

1. E.Hecht & A.R.Ganesan, Optics, Pearson, 2008

2. Jenkins and White, Fundamentals of Optics, TMH India, 4E, 2011

3. A K Ghatak, Introduction to Modern Optics, Tata-McGraw Hill, 4E, 2008

4. G R Fowles, Introduction to Modern Optics, Dover, 2E, 1989

22CHY282 **Basic Organic Qualitative Lab** **0 0 3 1**

Course Objective: To provide fundamental knowledge and hands on experience on functional group analysis of small organic compounds

Course Outcomes:

On successful completion of this course, a student will be able to

CO1: Capability in engaging in safe laboratory practices of handling laboratory glassware, equipment, and chemical reagents.

CO2: Ability to analyse systematically the functional group of a simple organic compound

CO3: Ability to characterize the analysed functional group with a derivative preparation.

Evaluation Pattern:

Assessment	**Internal**	**External**
Continuous Assessment (CA)*	80	
End Semester		20
Total	**100**	

1. Basic idea on the preparation of reagents used in organic analysis. (Borsches reagent, Schiff's reagent, phenolphthalein, neutral $FeCl_3$, Tollen's reagent, Fehling solution).
2. Determination of boiling point and melting point – capillary method.
3. Methods of re-crystallisation.
4. Tests for elements: nitrogen, halogens and sulphur.
5. Tests for unsaturation. Tests for aromatic character.
6. Study of the reactions of the following functional groups: alcohol, aldehyde, ketone, carboxylic acid, 1,2 dicarboxylic acid, ester, primary and secondary amines.
7. Systematic analysis of the following organic compounds containing one functional group and characterization with a derivative: alcohol, aldehyde, ketone, carboxylic acid, 1,2 dicarboxylic acid, ester, primary and secondary amines.

REFERENCES

1. *F. G. Mann and B. C. Saunders, 'Practical Organic Chemistry' 4th edition, Pearson Education, 2009.*
2. *V. K. Ahluwalia and S. Dhingra 'Comprehensive Practical Organic Chemistry' Universities Press, 2000.*
3. *B. S. Furnis, A. J. Hannaford, P. W. G. Smith and T. R. Tatchell, 'Vogel's Text book of Practical Organic Chemistry', ELBS/Longman, 1989.*
4. *S. P. Bhettani & Aruna Chhikara, 'Practical organic chemistry (qualitative analysis)', Ane books (India) Pvt Ltd, 2008.*
5. *O. P. Pandey, D.N Bajpai, S. Gini, 'Practical Chemistry, for I, II & III BSc. Students', S. Chand & Company Ltd reprint, 2009.*
6. *V. K. Ahluwalia, Sunitha Dhingra, Adarsh Gulate, 'College Practical Chemistry', Universities Press (India) Pvt Ltd, 2008.*

22CHY301 **Physical Chemistry III** **3 1 0 4**

Course Outcome:

On completion of the course the student will be able to

CO01: Understand the dual nature of electron, significance of the Schrodinger equation and its application.

CO02: Obtain knowledge about the symmetry of molecules, point groups and formation of Group multiplication table.

CO03: Acquire the knowledge of different statistical methods to derive the thermodynamic properties.

CO04: To understand and apply the concept of photophysical, photochemical reactions, photosensitized reaction and chemi-luminescence.

CO05: To acquire a sound knowledge about adsorption- types and mechanism and derivation of adsorption isotherms, colloids – types, preparation, properties and applications.

Evaluation Pattern:

Assessment	Internal	External
Periodical 1 (P1)	15	
Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	
End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1 Introduction to Quantum Chemistry

Introduction to quantum mechanics, Planck's quantum theory of radiation, photoelectric effect - dual nature of radiation, de Broglie's hypothesis - dual character of matter, uncertainty principle, Schrodinger wave equation - time dependent and time independent (no derivation), wave function ψ and its physical meaning, application of Schrodinger equation - particle in a one-dimensional box with two infinite potential barriers (energy of the particle, quantum number and quantization, momentum of the particle, energy level diagram, zero point energy, forms of the wave, node) and utility of this model, application of quantum mechanics to problems in chemistry - quantum chemistry (mention a few applications).

Unit 2 Basics of Group Theory

Symmetry- elements of symmetry and symmetry operations – identity, proper axis of rotation, plane of symmetry, improper axis of rotation and centre of inversion. Group and group theory- brief mathematical introduction, abelian and cyclic groups. Molecular point groups, classification and nomenclature of point groups- conditions and examples of non-axial, axial, dihedral and infinite point groups. Algebra of symmetry operations, matrix representations of symmetry operations, group multiplication table of C_2v and C_3v.

Unit 3 Irreversible and Statistical Thermodynamics

Reversible and irreversible thermodynamics, examples for irreversible processes, postulate or assumption of local equilibrium, entropy production - entropy production in heat flow and in matter flow, forces and fluxes, introduction to statistical thermodynamics, system, assembly, ensemble, canonical and micro canonical ensemble, Boltzmann distribution law (no derivation), partition function, qualitative and basic ideas of Maxwell-Boltzmann statistics, Bose-Einstein statistics and Fermi-Dirac statistics, bosons and fermions.

Unit 4 Photochemistry

Photochemistry - consequences of light absorption - Jablonski diagram – non-radiative transitions - radiative transitions – laws of photochemistry - Lambert's law, Beer's law and Beer-Lambert law, deviation from Beer's law, Grotthus-Draper law - the Stark-Einstein law of photochemical equivalence - quantum efficiency (quantum yield). Energy transfer in photochemical reactions – photosensitisation - photosynthesis in plants - chemiluminescence - fluorescence and phosphorescence – lasers - uses of lasers. Photochemical reactions - kinetics of hydrogen-bromine reaction, decomposition of HI, photoelectric cells, photosensitization and photosensitiser, photosynthesis.

Unit 5 Surface Chemistry and Colloids

Adsorption – physical and chemical - adsorption isotherms, Freundlich and Langmuir isotherms, positive, negative and electrostatic adsorption, applications of adsorption, colloidal state, dispersed phase, dispersion medium, types of colloidal systems, sols, gels and foams - lyophobic and lyophilic colloids, preparation by mechanical and electrical dispersion and chemical methods, purification by electrodialysis, and ultrafiltration, properties - colour, optical and electrical properties, qualitative idea of electrical double layer

(Helmholtz-Perrin theory, Gouy-Chapman theory, Stern's theory), stability of lyophobic and lyophilic sole, isoelectric point, protection of colloids - protective colloids. Gold Number, Hofmeister series, coagulation or flocculation - addition of electrolytes, continuous dialysis and salting out, Hardy-Schulze law, coacervation, sensitization, micelle and critical micellization concentration, application of colloids.

TEXTBOOKS

1. *R. K. Prasad, 'Quantum Chemistry', 3rd edition, New Age International Publishers, 2006.*
2. *Puri, Sharma &Pathania, 'Principles of Physical Chemistry', 42nd edition, Vishal Publishing Co, Delhi, 2007.*
3. *Gurdeep Raj, 'Advanced Physical Chemistry', 35th edition, Goel Publishing House, 2009.*

REFERENCES

1. *Donald A McQuarrie, "Quantum Chemistry", Viva Books Private Ltd.*
2. *Glasstone and Lewis, 'Elements of Physical Chemistry', 2nd edition, Macmillan, 1982.*
3. *R. Stephen Berry, Stuart A. Rice & John Ross, 'Physical Chemistry', 2nd edition, Oxford University press, 2000.*

22CHY302 Inorganic Chemistry III 3 1 0 4

Course Objective: To impart resonance familiarity on the advanced topics of inorganic polymers, supramolecules, chemistry of soil and nanomaterials.

Course Outcomes

CO1: Capacity to describe the chemistry of inorganic polymers and its commercial applications

CO2: Ability to understand the inorganic nanomaterials of gold, rhodium, palladium, platinum, iron, silver and carbon and their chemical synthesis

CO3: Capability to depict chemistry beyond the molecules through weak interaction and its application in supramolecular chemistry and molecular recognitions

CO4: Capacity to describe the basics of chemical aspects of soil

Skills: To provide wide knowledge in new chemistry of supramolecule and its application in molecular recognition in biological system.

Evaluation Pattern:

Assessment	**Internal**	**External**
Periodical 1 (P1)	15	
Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	
End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1 Inorganic Polymers

Properties of Inorganic polymers - silicones - composition, manufacture, structure properties and uses, silanes and their polymers, applications of phosphazenes, silicates and their polymers - classification into discrete anions - one-, two- and three-dimensional structures with examples - composition, properties and uses of beryl, asbestos, talc, mica, zeolites and ultramarines. **Metal Organic Frameworks** Introduction, porous coordination polymers, frameworks with high surface area, Lewis acid frameworks, soft porous crystals, design of metal organic frameworks and design of functional metal organic frameworks by post-synthetic modification, applications of metal organic frameworks

Unit 2 Inorganic Nanomaterials

General introduction to nanomaterials and emergence of nanotechnology; Moore's law; synthesis of nanoparticles of gold, rhodium, palladium, platinum, iron and silver; Synthesis of nanoparticle semiconductors, nanowires and nanorods; techniques of synthesis: electroplating and electrophoretic deposition, conversion through chemical reactions and lithography; thin films: chemical vapor deposition and atomic layer deposition techniques; carbon fullerenes and nanotubes - applications of nanoparticles.

Unit 3 Molecular Recognition

The concepts of molecular recognition, host - guest receptor systems. Forces involved in molecular recognition – hydrogen bonding, ionic bonding, p-stacking, van der Waal's and hydrophobic interaction.

Unit 4 Supramolecular Chemistry

Supra molecular Chemistry - Introduction to molecular receptors - design principles - tweezers, cryptands and carcerands – cyclophanes - cyclo dextrins and calixarenes - typical examples for molecular recognition and catalysis - catalysis by cation receptor, anion receptor and cyclophanes - molecular recognition in DNA and protein structure.

Unit 5 Non-aqueous Solvents

Classification of solvents – protic and aprotic solvents; acid, basic, and amphiprotic solvents, ionising and non-ionising solvents. Physical properties of solvents and their role in chemical reactions; types of reactions taking place in non-aqueous solvents – metathetical reactions, acid-base reactions, solvolytic reactions, oxidation-reduction reactions. Dielectric constant, activity coefficient, solubility. Reactions such as complex formation, precipitation, oxidation-reduction and acid type in non-aqueous solvents like liquid ammonia, liquid SO2 and liquid HF. Advantages and limitations of these solvents.

TEXT BOOKS

1. *F. A. Cotton, G. Wilkinson, C. A. Murillo & M. Bochmann, 'Advanced Inorganic Chemistry', 6th edition, John Wiley, 1999.*
2. *J.E. Huheey, 'Inorganic Chemistry - Principles, Structure and Reactivity', 4th edition, Harper Collins, New York, 1993.*
3. *Daji, A.J. 'A Textbook of Soil Science', Asia Publishing House, Madras, 1970.*

REFERENCE BOOKS

1. *Jonathan W. Stead, David R. Turner and karl. J. Wallace., 'Core concepts in Supramolecular Chemistry and Nanochemistry', John Wiley sons Ltd, 2007.*
2. *R. W. Hay, 'Bioinorganic chemistry', Halsted Press, 1984.*
3. *Tisdale, S.L., Nelson, W.L. and Beaton, J. D, 'Soil Fertility and Fertilizers', Macmillian Publishing Company, New York, 1990.*

22CHY303 Organic Chemistry II 3 1 0 4

CO 1. To understand the preparation and properties of organic compounds containing C-O and C-S bonds

CO 2. To familiarize the preparation and properties of carbonyl and sulphonyl compounds

CO 3. Discussion of the preparation and properties of active methylene compounds, enamines, and organometallic reagents

CO 4. Discussion of the preparation and properties of compounds containing nitro, amino and diazo functional groups

CO 5. Understand the classification, molecular structures, method of preparations and reactions of polycyclic and heterocyclic aromatic compounds

Evaluation Pattern:

Assessment	**Internal**	**External**
Periodical 1 (P1)	15	
Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	
End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1 Hydroxy Compounds, Ethers, Thioalcohols and Thioethers

Alcohols: nomenclature – preparation and properties. Monohydric alcohols: classification, physical properties - hydrogen bonding – distinction between primary, secondary, and tertiary alcohols, dihydric alcohols: oxidative cleavage - lead tetra acetate, periodic acid, pinacol - pinacolone rearrangements - mechanism**.**

Phenols: acidity of phenols, effects of substituents, comparison of acidity with alcohols. Preparation of nitrophenols, picric acid, catechol, resorcinol, and quinol. Mechanism of Reimer–Tiemann reaction, Lederer–Mannase reaction, Fries rearrangement

Ethers: nomenclature, preparation and reactions - Claisen rearrangement, Zeisel's method – crown ether structure.

Thioalcohols and thioethers - general physical and chemical characteristics. Synthesis of epoxides, cleavage of ether linkage by HI – Zeisel's method of estimation of alkoxy groups - Claisen rearrangement – mechanism. Thiols: mercaptans, methods of preparation, chemical properties, thioethers (basic idea only), mustard gas – structure, preparation and properties.

Unit 2 Carbonyl and Sulphonyl Compounds

Structure and reactivity of the carbonyl group- acidity of alpha hydrogen. Comparative studies of aldehydes and ketones, aliphatic and aromatic aldehydes - formaldehyde and acetaldehyde. Enols, enolates and reactions: Alkylation, kinetic and thermodynamic enolates, Aldol reaction, specific enol equivalents (lithium enolate, aza enolate, silyl enol ether, enamines, zinc enolates), Knoevenagel reaction, Perkin reaction, Reformatsky reactions, Cannizaro reaction, Mannich reaction, intramolecular aldol reaction, Acylation, Claisen condensation, Dieckman cyclization, Conjugate addition of enolates, Robinsons Annulation. Mechanism of nucleophilic additions to carbonyl groups with special emphasis on Claisen, Claisen–Schmidt, Benzoin, Aldol, Perkin, Favorskii, Fries, Dakin, Wittig rearrangements and Knoevenagel condensations. Condensations with ammonia and its derivatives, Wittig reaction, Mannich reaction, addition of Grignard reagents. Oxidation and reduction of aldehydes and ketones – Baeyer-Villiger oxidation – Cannizzaro's reaction, Meerwein–Pondorof-Verley reduction, Clemmensen reduction, Wolff-Kishner reduction, mechanism and selectivity in reduction of carbonyl compounds using $NaBH_4$, $LiAlH_4$ (including esters, amides and nitriles), and oxidation of alcohols using Jones, Collins, PCC, and PDC reagents, use of acetal as protecting group.

Structure of carboxylate ion – effects of substituents on acid strength of aliphatic and aromatic carboxylic acids – Hell–Volhard-Zelinsky reaction, mechanism of decarboxylation. Preparation of functional derivatives of carboxylic acids, acid chlorides, esters, anhydrides, and amides, their importance. Method of formation and chemical reactions of anthranilic acid, cinnamic acid, acrylic acid, oxalic acid, malonic acid, citric acid, adipic acid, fumaric acid and coumarin. Preparation and reactions of benzene sulphonic acid, benzene sulphonyl chloride and ortho, para toluene sulphonyl chlorides - uses.

Unit 3 Active Methylene Compounds, Enamines, and Organometallic Reagents

Preparation, reactions and structure of urea, thiourea and semicarbazide, manufacture of urea, preparation and basicity of guanidine. Compounds containing active methylene groups, synthetic uses of malonic ester, acetoacetic ester and cyanoacetic ester. Keto-enol tautomerism of ethyl acetoacetate, alkylation of carbonyl compounds via enamines. Structure and synthetic applications of alkyl lithium, butyl lithium, Grignard reagents, Reformatsky reaction.

Unit 4 Organic Compounds Containing Nitrogen

Nitro compounds – nomenclature, preparation and properties of aliphatic and aromatic nitro compounds. Reduction products of nitrobenzene in acidic, neutral and alkaline media, electrolytic reduction and selective reduction of polynitro compounds- formation of charge transfer complexes. Di- and tri- substituted aromatic nitro compounds – synthesis of o-, m-, p- dinitrobenzenes and trinitrobenzene.

Amino compounds – nomenclature and classification. Carbylamine reaction, diazotization – comparison of aliphatic and aromatic amines, stereochemistry of amines, reductive amination of aldehydic and ketonic compounds, Gabriel – Phthalimide reaction, Hoffmann bromamide reaction (mechanism needed). quaternary ammonium salts – phase transfer catalysis.

Diazonium salts – preparation and reactions. Azo coupling – mechanisms of Sandmeyers reaction, Gatterman reactions, Schiemann and Gomberg reactions Diazoalkanes and azides. Cyan compounds, preparation and uses of phenyl hydrazine, diazomethane and diazoacetic ester - synthetic uses- Arndt – Eistert synthesis – mechanism – Wolff rearrangement.

Unit 5 Polycyclic and Heterocyclic Aromatic Compounds

Classification, reactions and structure of naphthalene, anthracene and phenanthrene. Elementary idea of naphthyl amines, naphthols, naphthaquinone and anthraquinone.

Aromaticity of heterocyclic compounds (examples of each - 5 membered, 6 membered, and fused heterocycles, compound containing more than one hetero atom).

Five-membered heterocycles with one hetero atom – preparation and uses of furan, pyrrole, and thiophene. *Six-membered heterocycles with one hetero atom* - pyridines – synthesis. Quinoline and isoquinolines – synthesis with special references to Skraup, Bischler and Napieralskii and Fisher indole synthesis). Reaction mechanisms of electrophilic and nucleophilic substitutions, oxidation/reduction reactions. Resonance structures of heterocyclic compounds, applications. Fused ring heterocycles – synthesis, structure and reactivity.

TEXTBOOKS

1. *Morrison and R. N. Boyd, 'Organic Chemistry', 6th Edition, Prentice Hall, 1992.*
2. *K.S. Tewari and N.K. Vishnoi 'Organic Chemistry', 3rd Edition, Vikas Publishing House, 2005.*
3. *T.H. Lowry, K.S. Richardson, 'Mechanism and Theory in Organic Chemistry', 3rd edition, Harper Colins, New York, 1987.*

REFERENCES:

1. *L.G. Wade, J.R., 'Organic Chemistry', 5th edition, Pearson Education, Singapore, 2004.*
2. *Solomons & Fryhle, 'Organic Chemistry', 7th edition, Wiley India Pvt. Ltd., 2004. John McMurry, 'Fundamental of Organic Chemistry', 7th edition, Brook and Cole,*

22CHY381 Physical Chemistry Lab – Non-Instrumental 0 0 3 1

Course Outcome:

CO01: Acquiring skills in different methods of finding the molecular weights.
CO02: Acquiring knowledge on the concept of miscibility of liquids and perform the experiment.
CO03: Gaining knowledge on how impurity affects the physical characteristics of a compound and using that to find the CST, Eutectic temperature and molecular weight.
CO04: Imparting the skill in obtaining data and to derive the adsorption isotherm for adsorption processes.
CO05: Skillful performance of the experiments and to derive the kinetics of acid/base catalyzed ester hydrolysis.

Evaluation Pattern:

Assessment	Internal	External
Continuous Assessment (CA)*	80	
End Semester		20
Total	**100**	

1. Determination of CST of phenol-water system - effects of KCl/ NaCl salts on CST.
2. Phase diagram of simple eutectic system.
3. Determination of molecular weight of a high polymer by viscosity method.
4. Determination the molecular weight of a solute by Rast method using naphthalene or diphenyl as solvent using Beckmann thermometer.
5. Determination of the solubility of benzoic acid at different temperatures and ΔH of the dissolution process.
6. Determination of rate constant of acid catalyzed hydrolysis of an ester.
7. Adsorption of acetic acid from its aqueous solution by charcoal.
8. Determination of the distribution coefficient of iodine between water and carbon tetra chloride.
9. Determination of transition temperature of the given salt hydrate.

TEXTBOOKS

1. *R.C. Das and B. Behara, 'Experiments in Physical Chemistry', Tata McGraw-Hill, 1983.*
2. *Alexander Findlay,' Practical Physical Chemistry', 9th edition, Wiley, 1972.*

REFERENCES

1. *Gilbert William Castellan,' Physical Chemistry', Addison-Wesley Publishing Company, 1964.*
2. *James Brierley Firth, 'Practical Physical Chemistry', D. Van Nostrand Company, 1916.*

3. *Dr. J.B. Yadav, 'Advanced Practical Physical Chemistry', Krishna Prakashan Media, 29th edition, 2010.*

22CHY382 Organic Synthesis and Estimation Lab 0 0 3 1

Course Objective: To provide fundamental knowledge and hands on experience on functional group analysis of small organic compounds

Course Outcomes:

On successful completion of this course, a student will be able to

CO1: Able to calculate limiting reagent, theoretical yield, and percent yield of simple organic reactions.

CO2: Able to perform common laboratory techniques including titration, reflux, distillation, recrstallization, vacuum filtration, and thin-layer chromatography

CO3: capable of performing various one-step organic synthesis

Skill: This lab course imparts skill in calculating % yield, theoretical yield. To impart the knowledge of handing organic chemicals, and synthesis of organic compounds and basic separation techniques

Evaluation Pattern:

Assessment	Internal	External
Continuous Assessment (CA)*	80	
End Semester		20
Total	**100**	

1. Basic concepts on theoretical yield, practical yield, samples % conversion etc, Organic preparations including recrystallisation,
2. Synthesis of a) Acetanilide to p-nitroacetanilide b) Acetanilide to p-bromoacetanilide c) Benzyl chloride to benzoic acid, d) Nitrobenzene to dinitrobenzene e) Ester hydrolysis f) Benzoylation (phenol to phenyl benzoate);
3. Separation Techniques: Thin Layer Chromatography, Column chromatography

REFERENCES

1. *F. G. Mann and B. C. Saunders, 'Practical Organic Chemistry' 4th edition, Pearson Education, 2009.*
2. *V. K. Ahluwalia and S. Dhingra 'Comprehensive Practical Organic Chemistry' Universities Press, 2000.*
3. *B. S. Furnis, A. J. Hannaford, P. W. G. Smith and T. R. Tatchell, 'Vogel's Text book of Practical Organic Chemistry', ELBS/Longman, 1989.*
4. *O. P. Pandey, D.N Bajpai, S. Gini, 'Practical Chemistry, for I, II & III BSc. Students', S. Chand & Company Ltd reprint, 2009.*
5. *V. K. Ahluwalia, Sunitha Dhingra, Adarsh Gulate, 'College Practical Chemistry', Universities Press (India) Pvt Ltd, 2008.*

22CHY311 Basics of Analytical Chemistry 3 1 0 4

Course Objectives: To understand the basic principles behind the advanced analytical and separation techniques and interpretation of the analytical data.

Course Outcomes

COO1- Selecting a suitable analytical method for a specific purpose, and to evaluate sensitivity, sources of interference, errors, and apply analytical data in terms of statistics.

COO2 - Acquiring knowledge in contemporary separation methods and appropriate selection of instruments for the successful analysis of chemical compounds.

COO3 - Understanding the principle and working of the range of instrumental methods in analytical chemistry,

COO4 - Investigating solution behavior using electrochemical methods including potentiometry, conductometry, ion-selective, and cyclic voltammetric techniques.
COO5 - Apply different microscopic methods and XRD technique in the analysis of materials

Skill: Attaining skill in statistical analysis of data, separation techniques, Interpretation of data using XRD, TGA, DSC, Cyclic voltammetry.

Evaluation Pattern:

Assessment	Internal	External
Periodical 1 (P1)	15	
Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	
End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1 Theoretical Principles of Qualitative and Quantitative Analysis
Types of analytical methods - importance of analytical methods in qualitative and quantitative analysis - chemical and instrumental methods - advantages and limitations of chemical and instrumental methods. *Data Analysis* - types of errors, minimization of errors, propagation of errors, accuracy and precision, least square analysis, average standard deviation, coefficient of variance, significant figures, confidence interval, Q-test, t-test and F-test.

Unit 2 Chromatographic Techniques
Theory of separation, chromatographic separation, chromatographic techniques - column chromatography, thin layer chromatography, paper chromatography, ion-exchange chromatography, gas chromatography - principle, significance of R_f-values. HPLC, GC-MS, bioseparation - electrophoresis, centrifugation, DNA/protein separation, purification, polymer separation, green separation process, separation using zeolite and polymer membranes.

Unit 3 Thermal Analysis
Principle of thermogravimetry (TGA), differential thermal analysis (DTA), differential scanning calorimetry (DSC) - instrumentation and characteristics of TGA and DTA curves, factors affecting TGA and DTA curves. Applications - TGA of calcium oxalate monohydrate, DTA of calcium acetate monohydrate - determination of purity of pharmaceuticals by DSC, thermometric titrations.

Unit 4 Electro Analytical Techniques
Conductometry, ion selective electrodes. Potentiometry, amperometry, coulometry, polarography, voltammetry - cyclic voltammetry and anodic stripping voltammetry - principle and analysis of samples.

Unit 5 Crystallographic and Microscopic Techniques
XRD, X-ray crystallography, SAXD optical microscopy, scanning electron microscopy, transmission electron microscopy, scanning transmission electron microscopy, atomic force microscopy, AAS & ESCA

TEXTBOOKS

1. *Douglas A. Skoog and Donald M. West, F.J. Holler, 'Fundamentals of Analytical Chemistry', 7th edition, 7th edition, Saunders College publishers, 1995.*
2. *Usharani S., Analytical Chemistry, Macmillan, 2001.*

REFERENCES

1. *Mendham J., Denney R.C., Barnes J.D., Thomas M., 'Vogel's Text book of Quantitative Chemical analysis', 7th edition, Pearson education, 2008.*
2. *Sharma, B.K., 'Instrumental Methods of Chemical Analysis', Goel Publishing House, Meerut, 1997.*
3. *Gopalan. R., Subramaniam P.S. and Rangarajan. K., 'Elements of Analytical Chemistry', Sultan Chand and Sons, 2004.*

CO 1. To learn the configuration, method of preparation, and reactions and to elucidate the structure of mono, di and polysaccharides

CO 2. To explain the stereochemistry, structure, properties and biological roles of amino acids, peptides, proteins, and nucleic acids

CO 3. To understand the different classes, functions and mechanisms of vitamins, steroids, enzymes, and hormones

CO 4. To understand the field of natural products chemistry and lipids

CO 5. To learn synthetic methodologies, properties and application of dyes, synthetic polymers, soaps and detergents, paints and emulsions and food additives.

Evaluation Pattern:

Assessment	**Internal**	**External**
Periodical 1 (P1)	15	
Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	
End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1 Carbohydrates

Classification, constitution of glucose and fructose. Reactions of glucose and fructose, structure elucidation of fructose, osazone formation. Mutarotation and its mechanism, cyclic structure - pyranose and furanose forms. Determination of ring size. Haworth projection formulae, configuration of monosaccharides, epimerisation, chain lengthening and chain shortening of aldoses (Killiani – Fischer synthesis & Ruff degradation), interconversion of aldoses and ketoses, disaccharides – reactions and structure of sucrose, ring structure. Structure and properties of starch and cellulose (elementary idea only). Industrial applications of cellulose.

Unit 2 Amino acids, Peptides, Proteins and Nucleic acids

Amino acids: Sources of amino acids, classification, structure and stereochemistry of amino acids, preparation and reactions of α β, γ - amino acids, protection and deprotection of amino acids, essential and non-essential amino acids, zwitter ion, isoelectric point, C terminal and N terminal amino acids, functions of amino acids.

Peptides: structure, classification of peptides (linear, branched, cyclic, semicyclic), type of peptide bonds, characteristics, bioactive peptides, uses. Structure and function of vasopressin, oxytocin and hepcidin, dipeptides - biosynthesis, commercial dipeptides and its applications - aspartine, carnosine, acetyl carnosine, synthesis (carbo benzoxy method, Sheehan method), solution phase and solid phase peptide synthesis-Merrifield synthesis, designer peptides.

Proteins: - Structure of proteins, denaturation and colour reactions. Biosynthesis of protein, green fluorescent proteins

Nucleic acids: classification and structure of DNA and RNA. Replication of DNA, genetic codes.

Unit 3 Vitamins, Steroids, Enzymes, and Hormones

Vitamins - Classification and important sources, physiological action and deficiency symptoms of vitamin A, B_1, B_2, and B_{12}. C, D, E and K. Synthesis of ascorbic acid from glucose.

Steroids: Introduction- Diels hydrocarbon, structure and functions of cholesterol, elementary idea of HDL, LDL.

Enzymes: Chemical nature and properties of enzymes, nomenclature and classification of enzymes, mechanism of enzyme action, factors influencing the rate of enzyme kinetics, substrate specificity of enzymes, enzyme inhibition.

Hormones - introduction, classification, functions and mechanism of action of hormones

Unit 4 Terpenoids, Alkaloids, Lipids

Terpenoids (essential oils) - isoprene rule, structure elucidation of myrcene, citral and geraniol, natural rubber- structure, latex collection and treatment- vulcanisation.

Alkaloids: general methods of isolation, classification, general properties of alkaloids, exhaustive methylation, structure elucidation of conine, piperine, atropine and nicotine.

Lipids: biological functions- oils and fats, common fatty acids, extraction (Maceration, extraction using Soxhlet and Clevenger apparatus), refining, hydrogenation, rancidity, identification of oils and fats, saponification value, acid value, RM value, and iodine value

Unit 5 Organic Materials in Action

Synthetic polymers: synthesis and applications of polyesters- terephthalates, poly amides- Nylon 6 and Nylon 66, phenol – formaldehyde resins, urea formaldehyde resin, epoxy resins and polyurethanes, synthetic rubbers- SBR and nitrile rubber.

Dyes - preparation and uses of 1) Azo dye - Bismarck brown 2) Triphenylmethane dye - Malachite green 3) Phthalein dye - fluorescein 4) Vat dye – indigo 5) Anthraquinone dye- alizarin. Pigments – anthocyanins, flavones, phthalocyanines.

Soaps and detergents – composition of soaps - detergent action of soaps, synthetic detergents, their functions, comparison between soaps and detergents, LAS and ABS detergents.

Paints and Emulsions - **t**heir constituents and functions**.**

*Food Additives***:** artificial sweetening agents, food colours, emulsifying agents, preservatives, and leavening agents

TEXTBOOKS

1. *Morrison and R. N. Boyd, 'Organic Chemistry', 6th Edition, Prentice Hall, 1992.*
2. *I.L. Finar, "Organic Chemistry", 7th edition Vol I & II, Longman, 2009*
3. *S M Mukherji & S P Singh, "Reactions, Mechanisms of Organic Chemistry", 3rd edition, Macmillan Publishers India Ltd., 2009.*
4. *M. K Jain and S.C Sharma "Modern Organic Chemistry ' 3rd edition Vishal Pub company 2016*

REFERENCES

1. *L.G. Wade, J.R., 'Organic Chemistry', 5th edition, Pearson Education, Singapore, 2004.*
2. *Solomons and Fryhle, Organic Chemistry, 7th edition, Wiley India Pvt. Ltd., 2004.*
3. *John McMurry, 'Fundamentals of Organic Chemistry', 7th edition, Brook and Cole, 2011.*

22CHY313 Applied Organic Chemistry 3 1 0 4

CO 1. To learn about different medicinal agents

CO 2. Understand the concepts and methodologies applied in forensic chemistry

CO 3. Apply the knowledge of using computers and related techniques in studying organic chemistry processes

CO 4. Solve various types of problems related to organic chemistry

CO 5. Apply the knowledge of spectroscopy in solving the structures of simple organic compounds

Evaluation Pattern:

Assessment	**Internal**	**External**
Periodical 1 (P1)	15	
Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	
End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1 Chemotherapy

General introduction, classification of drugs, sulpha drugs, mode of action of sulpha drugs, uses. Antimalarials – chloroquine, primaquine, plasmoquin, proguanil, mepacrine. Antipyretics and analgesics- aspirin, methyl salicylate, paracetamol, phenacetin, phenyl butazone, analgin. Narcotics as analgesics - tranquilizers, antibiotics - penicillin, chloramphenicol, streptomycin, tetracyclines.

Unit 2 Forensic Chemistry

General introduction. Functions of forensic chemistry, definition and concepts in forensic science, scope, need and basic principles of forensic chemistry. Chemical toxicology - significance of toxicological findings, techniques used in toxicology, toxicological analyses and chemical intoxication tests, dose response relationship - LD50, ED 50, poisons, types, classification, physiochemical characteristics and mode of action of poisons, psychotropic substances, testing of narcotics, isolation and purification techniques for narcotics - TLC, GLC, HPLC, microcrystalline testing of drugs - DOPE test, heavy metal contamination of sea foods, use of neutron activation analysis for detecting arsenic in human hair,

explosives - classification, explosion process, blast waves, mechanism of explosion, detection of explosives. Significance of forensic chemistry

Unit 3 Computational Approaches in Organic Chemistry

Introduction, scope of computational chemistry, computational tools, molecular mechanics, molecular geometries, drawing chemical structures in chemdraw (acetylation reaction, condensation reactions), potential energy surfaces, local and global minima (calculation using scientific calculator), transition states. Isodesmic and homodesmic reactions - comparing ring strain energy of cycloalkanes. Cheminformatics- introduction, history and evolution of cheminformatics. Use and prospects of cheminformatics, molecular modelling (basic idea only) and structure elucidation. Application of cheminformatics in drug design.

Unit 4 Problem Solving Approaches in Organic Chemistry

Functional group interconversions- alcohol to aldehydes and carboxylic acids, nitro compounds to amines, carboxylic acids to its derivatives, cyanides to acids. Ascent and descent in – alcohol series, carboxylic acid series, interconversion of hexoses, reactions leading to isomerized products - pentanol isomer synthesis. Calculation of molecular formulae of organic compounds from percentage composition. Combustion analysis of alkanes - methane, butane, isopropane, cyclobutane and benzene. Thermal cracking reactions of hydrocarbons – pentane. Molecular weight determination of organic molecules - Victor Meyer method, silver salt method (problems expected). Ring formula – determination of unsaturation. Road map problems based on organic reactions.

Retrosynthesis: Introduction to retrosynthetic analysis

Unit 5 Applications of Organic Spectroscopy

IR, UV, and NMR spectral characteristics of simple molecules such as ethylene, butadiene, benzene, acetaldehyde, acetone, acetophenone, crotonaldehyde, ethanol, ethyl acetate, acetic acid, aniline, acetamide. Problems pertaining to the structure elucidation of simple organic compounds using IR, and PMR spectroscopic techniques, Mass spectrometry – introduction, EI ionization - determination of molecular mass by MS (elementary idea fragmentation study not required)

TEXTBOOKS

1. *T. Clark, Handbook of computational chemistry, Wiley, New York*
2. *AR. Leach, Molecular Modeling, Longman.*
3. *B.B. Nanda and R.K. Tiwari, Forensic Science in India: A Vision for the Twenty First Century, Select Publishers, New Delhi (2001).*
4. *S.H. James and J.J. Nordby, Forensic Science: An Introduction to Scientific and Investigative Techniques, 2nd Edition, CRC Press, Boca Raton (2005).*
5. *M. K Jain and S.C Sharma "Modern Organic Chemistry ' 3rd edition Vishal Pub company 2016*

REFERENCES

1. *L.G. Wade, J.R., 'Organic Chemistry', 5th edition, Pearson Education, Singapore, 2004.*
2. *Solomons and Fryhle, Organic Chemistry, 7th edition, Wiley India Pvt. Ltd., 2004.*
3. *John McMurry, 'Fundamentals of Organic Chemistry', 7th edition, Brook and Cole, 2011.*
4. *D.E. Zulawski and D.E. Wicklander, Practical Aspects of Interview and Interrogation, CRC Press, Boca Raton (2002).*

5. *R. Saferstein, Criminalistics, 8th Edition, Prentice Hall, New Jersey (2004).*
6. *J.L. Jackson and E. Barkley, Offender Profiling: Theory, Research and Practice, Wiley, Chichester (1997).*
7. *M. Byrd, Crime Scene Evidence: A Guide to the Recovery and Collection of Physical Evidence, CRC Press, Boca Raton (2001).*
8. *W.J. Tilstone, M.L. Hastrup and C. Hald, Fisher's, Techniques of Crime Scene Investigation, CRC Press, Boca Raton (2013)*

22CHY314 Basic Spectroscopic Techniques 3 1 0 4

Course Objective: To impart sound knowledge on the theoretical aspects and practical interpretation skill for the structure of small organic molecules using 1H and 13C NMR and mass spectra.

Course Outcome

CO1: Capacity to understand and imply the knowledge of electromagnetic radiation in spectroscopy techniques

CO2: Ability to demonstrate the functional group analysis, both quantitative and qualitative analysis of small organic molecules and coordination compounds.

CO3: Capability to interpret the structure of small organic molecules using 1H and 13C NMR and EI - mass spectra

Evaluation Pattern:

Assessment	Internal	External
Periodical 1 (P1)	15	
Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	
End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1 Electromagnetic Spectrum

Introduction – definition of spectrum – electromagnetic radiation – regions of spectrum, quantization of different forms of energies in molecules (translational, rotational, vibrational and electronic) - Born Oppenheimer approximation.

Unit 2 Electronic Spectroscopy

Principle – absorption laws. Calculations involving Beer Lamberts' law – instrumentation - photo colorimeter and spectrophotometer - block diagrams with description of components - theory - type of electronic transitions - chromophore and auxochromes – absorption bands and intensity – factors governing absorption maximum and intensity. Calculation of λ_{max} using Woodward Fischer rule for simple molecules.

Unit 3 Vibrational Spectroscopy

Principle - vibrational frequency - fundamental vibrations – modes of vibration of diatomic, triatomic linear (CO_2) and nonlinear triatomic molecules (H_2O) - stretching and bending vibrations - selection rules. Hooke's law. Instrumentation - sampling techniques. Applications of IR spectroscopy - interpretation of the spectra of alcohols, aldehydes, ketones and esters – aliphatic and aromatic.

Unit 4 NMR Spectroscopy

Principle of nuclear magnetic resonance – basic instrumentation – number of signals - chemical shift – shielding and deshielding. Spin-spin coupling and coupling constants. TMS as NMR standard. Introduction to H^1 and C^{13} NMR spectrum. Interpretation of proton NMR spectra of simple organic compounds such as

acetone, anisole, benzaldehyde, ethyl acetate, ethylamine, ethyl bromide, toluene and isopropyl phenyl ketone.

Unit 5 Mass Spectrometry

Basic principles – instrumentation – molecular ion peak, base peak, metastable peak, isotopic peak their uses. Fragmentation pattern – nitrogen rules- determination of molecular formulae – types of mass analysis. Interpretation of mass spectra of simple organic compounds such as acetone, anisole, benzaldehyde, ethyl acetate, ethyl amine, ethyl bromide, toluene and isopropyl ketone. Mc-Lafferty Rearrangement.

TEXTBOOKS

1. *P.S. Kalsi 'Spectroscopy of organic Compounds', 6th edition, New age international publishers, 2005.*
2. *W. Kemp, 'Organic Spectroscopy, Macmillan, 1987*

REFERENCES

1. *R.M. Silverstein, F. Webster and D. Kimle 'Spectroscopic Identification of Organic Compounds 7th edition, 7 Wiley and Sons, 2005.*
2. *C.N. Banwell 'Fundamentals of Molecular Spectroscopy' 4th edition, McGraw –Hill College, 1994.*
3. *Dyer Jhon R, 'Applications of Absorption Spectroscopy of Organic Compounds', PHI learning Publishers, 1965.*

22CHY383 Inorganic Quantitative Lab- Gravimetric Analysis 0 0 5 2

Course Objective: To develop basic skills in performing quantitative analysis of samples by gravimetric methods.

Course Outcome:

After completing this course successfully, the student will be able to,

CO01: Express a sound knowledge in calculations based on mole concept.
CO02: Perform gravimetric estimation of metals, by utilizing precipitation principles and filtration techniques for metal salts and oxides.
CO03: Perform gravimetric estimation of metals, by utilizing precipitation principles and filtration techniques for metal complexes (co-ordination compounds)
CO04: Analyse the composition of alloys using gravimetric method.

Evaluation Pattern:

Assessment	Internal	External
Continuous Assessment (CA)*	80	
End Semester		20
Total	**100**	

1. Gravimetric estimation of barium as barium sulphate.
2. Gravimetric estimation of iron as iron (III) oxide.
3. Estimation of sulphate as barium sulphate.
4. Gravimetric estimation of copper as copper (I) thiocyanate.
5. Gravimetric estimation of nickel as nickel dimethylglyoximate.
6. Gravimetric estimation of magnesium as magnesium 8-hydroxy quinolate
7. Estimation of iron in the given sample of haematite by dichromate method.
8. Estimation of copper in bronze by iodometric method.
9. Estimation of tin in solder using EDTA.

TEXTBOOKS

1. *G.H. Jeffery, J. Bassett, J. Mendham and R.C. Denny 'Vogel's Text Book of Quantitative Chemical Analysis', 5th Edition, ELBS, 1989.*
2. *D.A. Skoog and D.M. West 'Analytical Chemistry-An Introduction', 4th Edition, CBS Publishing Japan Ltd., 1986.*

REFERENCES

1. *E.J. Meehan, S. Bruckenstein and I.M. Kolthoff and E.B. Sandell, 'Quantitative Chemical Analysis', 4th Edition, The Macmillan Company, 1969.*
2. *R.A. Day (Jr) and A.L. Underwood, 'Quantitative Analysis', 6th Edition, Prentice Hall of India, 1991.*

22CHY384 Physical Chemistry Lab: Instrumental 0 0 5 2

Course Objective:

CO01 Understand the usage of different analytical instruments

CO02 Apply the principles of electrolyte conductance and electrode potential for analytical applications.

CO03 Evaluate the optical properties of chemical species and explore its analytical applications.

Evaluation Pattern:

Assessment	Internal	External
Continuous Assessment (CA)*	80	
End Semester		20
Total	**100**	

1. Determination of cell constant and equivalent conductivities of different electrolyte by conductometry.
2. Determination of the strength of strong and weak acids in a given mixture conductometrically.
3. Determination of the velocity constant, order of the reaction and energy of activation for saponification of ethyl acetate by sodium hydroxide, conductometrically.
4. Determination of solubility and solubility product of sparingly soluble salt (e.g. $PbSO_4$, $BaSO_4$) conductometrically.
5. Determination of the strength of strong and weak acids in a given mixture using a potentiometer.
6. Determination of the strength of strong and weak acids in a given mixture using a pHmeter..
7. Determination of pK_a of acetic acid using pH meter.
8. Determination of concentration of an electrolyte by Nernst equation.
9. Potentiometric redox titration of ferrous ion with potassium dichromate.
10. Verification of Beer – Lambert's law. Determination of unknown concentration using colorimeter
11. Determination of concentration of ions by Spectrophotometer.
12. Determination of concentration of potassium and sodium ion by flame photometry.
13. Determination of transport number of silver ion.

TEXTBOOKS

1. *R.C. Das and B. Behara, 'Experiments in Physical Chemistry', Tata McGraw-Hill, 1983.*
2. *Alexander Findlay,' Practical Physical Chemistry', 9th edition, Wiley, 1972.*

REFERENCES

1. *Gilbert William Castellan,' Physical Chemistry', Addison-Wesley Publishing Company, 1964.*
2. *James Brierley Firth, 'Practical Physical Chemistry', D. Van Nostrand Company, 1916.*
3. *Dr. J.B. Yadav, 'Advanced Practical Physical Chemistry', Krishna Prakashan Media, 29th edition, 2010.*

22CHY331 Batteries and Fuel Cells 3 0 0 3

CO1: Get the knowledge about fundamentals of electrochemistry which involves origin of potential, calculation of EMF of cell, Nernst equation etc.

CO2: Awareness on types, working, applied areas, advantages as well as disadvantages of primary and secondary batteries.

CO3: Awareness on types and working of fuel cells.

CO4: Understanding how to establish a relationship with industries by excercising applied science.

Evaluation Pattern:

Assessment	Internal	External
Periodical 1 (P1)	15	
Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	
End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1 Background Theory

Origin of potential - electrical double layer - reversible electrode potential - standard hydrogen electrode - emf series - measurement of potential - reference electrodes (calomel and silver/silver chloride) indicator and ion selective electrodes - Nernst equation - irreversible processes - kinetic treatment - Butler-Volmer equation - overpotential, activation, concentration and IR overpotential - its practical significance - Tafel equation and Tafel plots - exchange current density and transfer coefficients**.**

Unit 2 Batteries: Primary Batteries

The chemistry, fabrication and performance aspects, packing classification and rating of the following batteries: (The materials taken, their function and significance, reactions with equations, their performance in terms of discharge, capacity, and energy density to be dealt with). Zinc-carbon (Leclanche type), zinc alkaline (Duracell), zinc/air batteries; Lithium primary cells - liquid cathode, solid cathode and lithium-ferrous sulphide cells (comparative account).

Unit 3 Secondary Batteries

Lead acid and VRLA (valve regulated (sealed) lead acid), nickel-cadmium, nickel-zinc, nickel-metal hydride batteries, lithium-ion batteries, ultrathin lithium polymer cells (comparative account). Advanced batteries for electric vehicles, requirements of the battery - sodium-beta and redox batteries**.**

Unit 4 Fuel Cells

Description, working, principle, anodic, cathodic and cell reactions, fabrication of electrodes and other components, applications, advantages, disadvantages and environmental aspects of the following types of fuel cells: proton exchange membrane fuel cells, alkaline fuel cells, phosphoric acid, solid oxide, molten carbonate, direct methanol fuel cells. Membranes for fuel cells: Nafion – Polymer blends and composite membranes; assessment of performance – recent developments.

Unit 5 Fuels for Fuel Cells

Hydrogen, methane, methanol - sources and preparation, reformation processes for hydrogen – clean up and storage of the fuels – use in cells, advantages and disadvantages of using hydrogen as fuel.

TEXTBOOKS

1. *Dell, Ronald M Rand, David AJ, 'Understanding Batteries', Royal Society of Chemistry, (2001).*
2. *M. Aulice Scibioh and B. Viswanathan 'Fuel Cells – principles and applications', University Press, India (2006).*

REFERENCES

1. *Kanani N, 'Electroplating and electroless plating of copper and its alloy', ASM International, Metals Park, OH and Metal Finishing Publications, Stevenage, UK (2003).*
2. *Curtis, 'Electroforming', London, (2004).*
3. *F. Barbir, 'PEM fuel cells: theory and practice', Elsevier, Burlington, MA, (2005).*
4. *G. Hoogers, 'Fuel cell handbook', CRC, Boca Raton, FL, (2003).*

22CHY332 Corrosion Science 3 0 0 3

Course Objective: To introduce the students to the underlying science of corrosion, thermodynamic and kinetic principles, mass transfer and potential theory, the causes, mechanism and prevention methods of various types of corrosion, its measurement and combating methods.

Course outcomes

On completion of the course the student will be able to

CO1: Understand the fundamentals of corrosion reactions and their mechanism

CO2: Identify the forms of corrosion

CO3: Evaluate corrosion rate and passivation potential

CO4: Provide methods for protection of materials

CO5: Select a suitable material for a specific application

Evaluation Pattern:

Assessment	Internal	External
Periodical 1 (P1)	15	
Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	
End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1 Introduction to Corrosion
Mechanisms of Chemical corrosion, electrochemical corrosion, concentration cell corrosion, pitting corrosion, intergranular corrosion, waterline corrosion, stress corrosion.

Unit 2 Cathodic Protection
Basis of cathodic protection, working of cathodic protection, electrochemical theory of cathodic protection, design parameters in cathodic protection, cathodic protection interferences.

Unit 3 Corrosion Kinetics
Faradays laws of electrolysis and its application in determining corrosion rates, the laws, corrosion kinetics, mixed potential theory and its application, resistance polarization, determination of corrosion rates by electrochemical measurements, kinetics of passivity.

Unit 4 Corrosion Prevention by Design
Corrosive environment, stages in design processes, soldering and threading, crevices, flowing water systems, design for liquid containers, design in packaging, coating and design, storage of combat vehicles.

Unit 5 Selection of Materials for Corrosive Environment
Factors affecting the performance of materials, materials classification, materials and fluid corrosivity, corrosion behaviour of several materials.

TEXTBOOKS

1. *Mars G. Fontana, 'Corrosion Engineering', 3rd edition, Tata McGraw-Hill, 2005.*
2. *P.E. Philip A. Schweitzer, 'Corrosion Engineering Handbook', 2nd edition, Inco alloys International, 1996.*

REFERENCES

1. *R. Winston Revie and Herbert H Uhlig, 'Corrosion and Corrosion Control', 4th edition, John Wiley & Sons, 2008.*
2. *Zaki Ahmad, 'Principles of Corrosion Engineering and corrosion', 3rd edition John Wiley & Sons, 2006.*

22CHY333 Green Chemistry 3 0 0 3

Course Outcomes
On successful completion of this course, a student will be able to

CO1: Develop fundamental understanding of the principles of Green Chemistry and a quantitative estimation of greenness of a chemical reaction through sustainability metrices.
CO2: Understand the alternate solvents systems and green solvents available for application in industrial reactions.
CO3: Analyze industrial catalytic processes regarding sustainability.

Skill development: Innovation is the call of the day and green chemistry will help develop requisite skills for innovative reaction schemes for sustainable applications.

Evaluation Pattern:

Assessment	Internal	External

Periodical 1 (P1)	15	
Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	
End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1 Introduction to Green Chemistry

Introduction - inception and evolution of green chemistry - principles of green chemistry - the green chemistry expert systems - the measure of greenness - safety and risk indices - the hierarchical approach - green chemistry and sustainable development - pollution control to pollution prevention - Indian perspective on green chemistry - information technology and sustainable development.

Unit 2 Green Reagents

Green reagents - safer solvents - green solvents - water as a solvent - solvent free conditions - support reagents - ionic liquids and their applications - super critical systems (CO_2) as green solvents - hydrogen peroxide in green oxidation reactions - dimethyl carbonate, a green solvent and an ambient reagent.

Unit 3 Green Chemical Techniques I

Environmentally benign technologies by green chemistry (with examples) - microwave assisted synthesis - electro-organic synthesis - photochemical degradation as a green approach for waste treatment - catalysis and green chemistry - supported catalysts and reagents for green chemistry - heterogenized reactions for green chemistry - oxidation technology for waste water treatment - green chemistry using biocatalytic reactions.

Unit 4 Green Chemical Techniques II

Aqueous phase reactions, solid state reactions, enzymatic transformations, sonicated reactions - usual organic reactions (Benzoin condensation, Michael Addition, Heck Reaction, Darzen reaction, Heck reaction, Claisen arrangement) in a greener way.

Unit 5 Green Industrial Processes and Operations

Cleaner production - industrial perspectives - reactions and reactor designs - micromixers - unit operations - reactions with separation processes alternate energy resources - inherent safety - green chemistry and industries - the pharmaceutical industries and green chemistry - the polymer industry - pesticides, antifoulants, and herbicides - solvents and green chemistry - the food and flavor industry - the maleic anhydride manufacturing process - chelants - the surfactant industry - industries in need of support to go green - the semiconductor manufacture industry - the dye industry - the textile industry - the tannery industry - the sugar and distillery industries - the paper and pulp industry - the paint industry - Green chemistry in future.

TEXTBOOKS

1. *Mukesh Doble and Anilkumar Kruthiventi, 'Green Chemistry and Processes', reprint, Science Press, 2007.*
2. *Paul T. Anastas and Tracy C. Williamson, 'Green chemistry: frontiers in benign chemical syntheses and processes', Oxford University Press, 1998.*

REFERENCES

1. *V. K. Ahluwalia, 'Green Chemistry - Environmentally Benign Reactions', 1st edition, Ane Books Pvt Ltd, 2009.*
2. *M. M. Srivastava, Rashmi Sanghi, 'Green Chemistry - Environment Friendly Alternatives', 2nd edition, Narosa Publishing House, 2005.*

22CHY334 Industrial Catalysis 3 0 0 3

Course Objective: To impart basic knowledge on different types of catalysts and their industrial application.

Course Outcome:

CO1: To develop knowledge on chemical aspects of catalysis

CO2: Able to understand the different classification of catalysts

CO3: To understand the importance and preparative methods industrial catalysis process

Skills: To provide beginner knowledge in new chemistry of catalysis and its application in industry.

Evaluation Pattern:

Assessment	Internal	External
Periodical 1 (P1)	15	
Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	
End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1 Catalysis

An introduction, general principles of catalysis, activation energy plots for catalytic processes, classification for catalysis - heterogeneous and homogeneous catalysis, van't-Hoff's and Arrhenius treatment of homogeneous catalysis - kinetic aspects, adsorption and general principles of heterogeneous catalysis - kinetic aspects, determination of surface area and pore-structure of the catalyst, definition of performance criteria of catalysts, activity, selectivity, temperature response, catalyst life.

Unit 2 Catalysis in Solutions

Acid and base catalysis, catalysis in gas phase, catalysis in dilute aqueous solutions, catalysis in concentrated strong acid solutions, catalysis by bases, catalysis by metal ions, electron transfer catalysis, catalysis by co-ordination and organometallic compounds, catalysis in Ziegler-Natta, metallocene, metathesis, catalysis by enzymes.

Unit 3 Polymers and Zeolites in Catalysis

Catalysis by polymers, polymer supported catalysts, catalysis in polymer gels, phase transfer catalysis, catalysis in molecular scale cavities, zeolites - molecular sieves, shape selective and size selective catalysis

Unit 4 Catalysis by Metals, Metal Oxides and Supported Metals

Electronic factors in catalysis by metals, valence bond and electron band theories, electronic factors in catalysis by semiconductors, co-operative electronics interactions and catalysis, localized interactions and catalysis, surface states and catalysis, role of supports, preparation and structure of supports, silica, alumina, silica-alumina, carbon, monolithic supports, surface properties, catalyst manufacture, catalyst size and shape, pre-treatments, deactivation processes, sintering, poisoning and catalyst fouling.

Unit 5 Industrially Important Catalytic Processes

Catalysis and green chemistry, catalysis by ionic liquids, catalytic reforming, catalytic cracking, hydrotreatment, steam cracking, Fisher Tropsch process, mobile process for conversion of methanol to gasoline hydrocarbons, catalysis for environmental protection, removal of pollutants from exhausts, mobile and static sources, effluent clean up analysis, applications in the production of fertilizers, acetic acid, formaldehyde, washing powder additives, pharmaceuticals.

TEXTBOOKS

1. *Bruce G Gates, 'Catalytic Chemistry', John Wiley & Sons, 1992.*
2. *J. A. Jensen, K. B. Rider, Y. Chen, M. Salmeron and G. A. Somorjai and E. K. Rideal, 'Concepts in Catalysis', Academic Press, New York, 1968.*
3. *Alfred Clark, 'The Theory of Adsorption and Catalysis', Academic Press, 1970.*

REFERENCES

1. *W.B. Innes, 'Experimental Methods in Catalytic Research', Volume 1, R.B. Anderson Academic Press, 1968.*
2. *J.M. Betty, 'Applied Industrial Catalysis', Volume 1, Academic Press, 1983.*
3. *Ronald Pearce, William R. Patterson, 'Catalysts and Chemical Processes', Wiley, 1981.*
4. *Michael Bowker, 'The Basis and Applications of Heterogeneous Catalysis', Oxford University Press,*

1998.
5. *J.C. Kuriakose, 'Catalysis', Macmillan India LTD, 1991.*
6. *Calvin H. Bartholomew and Robert J. Farrauto, "Fundamentals of Industrial Catalysis"*

22CHY335 Introduction to Food Chemistry 3 0 0 3

Course Outcome:

CO1: Understand major and minor foods and their physical states.
CO2: Enlist the properties of water and its role in food system.
CO3: Understand the properties of Carbohydrates and proteins and its role in food system.
CO4: Comprehend the properties of Lipids, Vitamins and Minerals and its role in food system.
CO5: Ability to describe the basic properties and functions of enzymes, pigments, food additives its role in food system.
Skills: To provide an understanding of the chemical interactions of food components and their effects on sensory and nutritional quality, functional properties, and safety of foods

Evaluation Pattern:

Assessment	Internal	External
Periodical 1 (P1)	15	
Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	
End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1 Introduction

Definition of food, major components of food, physical states of food – dispersions, true solutions, colloidal, emulsions, foam and gel, factors affecting stable dispersion of food ingredients, functions of emulsifiers and stabilizers. Water - **f**unctions of water in food systems, hydrogen bonds, permanent dipole moment dielectric constant, theories of solvent action, water activity and food stability, absorption isotherm curve, roles of water in physical properties and chemical reactions in food theories and applications of different moisture determination methods.

Unit 2 Proteins and Carbohydrates

Protein **-** Classifications, nomenclature, and structures of aminoacids, basic properties of protein, structure of proteins, protein functional groups and their chemical, hydrophobic, and hydrophobic properties, isoelelctric point and solubility as a function of pH, protein denaturation and its effects on food systems, nutritional quality of protein, theories & applications of analytical methods for protein and amino acids determination.

Carbohydrates **-** Classification, nomenclature, and structures of Carbohydrates, isomers and absolute configurations of Carbohydrates, physical – chemical properties of Carbohydrates, sweetness of Carbohydrates, functions of Carbohydrates in foods, chemical reactions of Carbohydrates, analytical methods for Carbohydrate determination.

Unit 3 Lipids and minerals

Lipids **-** Nomenclature and structures of fatty acids, classifications of lipids, physical and chemical characteristics of different fats, relationship between chemical structure and fat melting properties, analytical methods for determining different physical and chemical characteristics of fat, lipid oxidation mechanisms, principles and applications of analytical methods for the determination of fat content and fatty acid composotions of foods.

Minerals **-** Ash determination methods, principles and applications of different methods for determining individual minerals – atomic absorption and flame spectrometry's, and chemical methods.

Unit 4 Vitamins

Water soluble and fat soluble vitamins, chemical reactions and losses of vitamins during processing and storage. Principles and techniques for the determination.

Unit 5

Pigments in food flavours, browing reaction in foods, enzymes in foods, and food industry, bio-

deterioration of foods, food contaminants, food additives and toxin.

REFERENCE

Fennema's Food Chemistry fourth edition,edited by S. Damodaran, K.L. Parkin, and O.R Fennema, 2007 published by CRC Press .

SUGGESTED READINGS

1. *Aurand, L.W. and Woods, A.E. 1973. Food Chemistry. AVI, Westport*
2. *Birch, G.G., Cameron, A.G. and Spencer, M.1986. Food Science, 3rd ED.Pergamon Press, New york.*
3. *Fennema O.R. Ed. 1976. Principles of Food Science: Part – I Food Chemistry. Marcel Dekker, New york.*
4. *Meyer, L.H. 1973. Food Chemistry. East – West Press Pvt. Ltd., New Delhi.*
5. *Potter, N.N. 1978. Food Science. 3rd Ed. AVI, Westport*

22CHY336 Polymer Chemistry 3 0 0 3

Evaluation Pattern:

Assessment	Internal	External
Periodical 1 (P1)	15	
Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	
End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1 Introduction to Polymers and Polymerization

History of polymer Science. Concept of macromolecules, nomenclature and classification. Polymer, monomer, oligomer, repeating unit, degree of polymerization, functionality, copolymer - random, alternating, graft, block, tacticity. polymerization processes. Free radical addition polymerization- kinetics and mechanism. Chain transfer. Mayo-walling equation of the steady state. Molecular weight distribution and molecular weight control. Radical atom transfer and. fragmentation – addition mechanism. Free radical living polymers. Cationic and anionic polymerization. Kinetics and mechanism, polymerization without termination. Living polymers. Step Growth polymerization- kinetics and mechanism. Molecular weight distribution. Linear vs cyclic polymerization, other modes of polymerization. Group Transfer, metathesis and ring opening polymerization. Copolymerization. The copolymerization equation, Q-e scheme, gelation and cross linking. Copolymer composition drifts, polymerization techniques - bulk solution, melt, suspension, emulsion, and dispersion techniques.

Unit 2 Polymer Stereochemistry and Characterization

Organizational features of polymer chains. Configuration and conformation, tacticity, repeating units with more than one asymmetric center. Chiral polymers - main chain and side chain. Stereo regular polymers. Manipulation of polymerization processes. Zeigler-Natta and Kaminsky routes. Coordination polymerization. Metallocene and metal oxide catalysts. Polymer characterization. Molecular weights. Concept of average molecular weights, Molecular weight distribution. Methods for determining molecular weights. Static and dynamic methods, light scattering and GPC. Crystalline and amorphous states. Glassy and rubbery states. Glass transition and crystalline melting. Spherulites and lamellar. Degree of crystallinity, X-ray diffraction, thermal analysis of polymers. TG/DTG, DTA/DSC, DMA/TMA/DMTA. Spectroscopy of polymers. Microstructure determination by IR, Raman, UV, NMR and MS techniques. Solid state NMR and polymer stereochemistry. Structure-property relationship. Elastomeric and viscoelastic states. Rubber-like elasticity. Maxwell and kinetic model of viscoelasticity.

Unit 3 Polymer Solutions

Treatment of dilute solution data. Thermodynamics. Flory-Huggin's equation. Chain dimension - chain stiffness - end-to-end distance. Conformation-random coil, solvation and swelling. Flory-Reiner equation. Determination of degree of cross linking and molecular weight between crosslinks. Polymer structure - property relationship, crystalline and amorphous combinations.

Unit 4 Polymer Additives, Blends and Composites

Introduction - general principles, use of additives to enhance and protect properties of polymer, classes of polymer additives - type, structure, chemistry, mechanism and suitability: for antioxidant-heat stabilizers - UV stabilizers - HAL-antistatic - blowing agents - lubricants nucleating agents - cross linking agent - flame retardant-compatibiliser. Fillers - effect and type of fillers - surface treatment and coupling agent. Coloration of polymers – pigment - colour measurement. Plasticizer – function - mode of operation - types. Compounding - main types of colorants – equipments - internal mixer, two roll mill, Banbury mixer, single screw extruder, twin screw extruder - co rotating - counter rotating - intermeshing. Fabrication methods, polymer blends, toughened plastics and phase separated blends, interpenetrating network, mechanical properties, composite fabrication.

Unit 5 Industrial and Speciality Polymers

Synthesis, structure and applications of polyethylene, polypropylene, polystyrene. Homo and copolymers. Diene rubbers. Vinyl and acrylic polymers. PVC, PVA, PAN, PA. poly (vinyl carbazole), poly (vinyl imidazole). PMMA and related polymers. Copolymers. EVA polymers. Fluorine containing polymers. Polyacetals. Reaction polymers. Polyamides, polyesters. epoxides, polyurethanes, polycarbonates, phenolics, PEEK, silicone polymers. Reactions of polymers. Polymers as aids in Organic synthesis. Polymeric reagents, catalysts, substrates, liquid crystalline polymers. Main chain and side chain liquid crystalline polymers. Phase morphology. Conducting polymers. Polymers with high bandwidth. Polyanilines, polypyrrols, polythiophenes, poly (vinylene phenylene). Photoresponsive and photorefractive polymers. Polymers in optical lithography. Polymer photo resists. Electrical properties of polymers, polymers with NLO properties, second and third harmonic generation, and wave guide devises.

TEXTBOOKS

1. *F.W. Billmayer, 'Textbook of Polymer Science', 3rd Edition, Wiley. N.Y. 1991.*
2. *J.M.G Cowie, 'Polymers: Physics and Chemistry of Modern Materials', 2nd edition, Blackie Academic and professional, 1991.*
3. *P.J. Flory, 'Principles of polymer chemistry', reprint, Cornell University Press, 1953.*

REFERENCES

1. *F. Ullrich, 'Industrial Polymers', Kluwer, N.Y. 1993.*
2. *H.G. Elias, 'Macromolecules, Vol. I & II', Academic, 1991.*
3. *Harry A Allcock, Frederick W Lampe and James E Mark, 'Contemporary Polymer Chemistry', 3rd edition, Pearson Prentice Hall, 2003.*

22CHY337 Surface Science and Coating Technology 3 0 0 3

Evaluation Pattern:

Assessment	Internal	External
Periodical 1 (P1)	15	
Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	
End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1 Introduction to Paints and Paint Technology

General introduction to paint industry - definition of paints, varnishes and lacquers their constitution and functions, general classification of surface coatings - decorative and protective coatings - paint industries in India.

Unit 2 Pigments Dyes and Extenders

Definition and classification of pigments and dyes - properties and evaluation of pigments such as crystal structure particle size and shape, refractive index and hiding power, oil absorption, colour, specific gravity and bulking value, UV and IR absorption, light fastness, resistance to heat water, alkali and acid, corrosion inhibition, toxicity, reducing power, tinting strength, flooding and floating, settling, volatile and water soluble matter, residue on sieve, bleeding - white pigments and coloured pigments - organic and inorganic

pigments - industrial manufacture of pigments - special effect pigments - Extenders - use and functions of extenders - examples for extenders.

Unit 3 Binding Media, Solvents and Additives in Paints

Fundamentals of film formers, chemical structure of monomers, functionality and its determination, degree of polymerization and molecular weight, non-convertible and convertible film formers, linear, branched and cross linked film formers, homopolymers and copolymers - manufacture, chemistry and applications of alkyd resins, polyester resins, phenolic resins, amino resins, epoxy resins, polyamide resins, polyurethanes, silicone resins, vinyl and acrylic resins - emulsions - polystyrene and styrene-acrylic emulsions. Solvents, dryers, surfactants and other additives in paints.

Unit 4 Paint Formulation, Manufacture and Application Techniques

Principles of paint formulation, formulation elements, mathematics & steps: PVC, CM, P/B ratio, sp gravity, etc; typical formulations of primers, undercoats and finish coats - steps in paint manufacturing, phenomenon of wetting, grinding and dispersion, important considerations in pigment dispersion and rheology - different milling and mixing techniques - factors affecting effectiveness of milling such as size, speed and type of mill; volume, composition, size and shape of grinding medium - mill base. Surface preparation techniques - physical and chemical surface treatment techniques - common application techniques - packaging technology.

Unit 5 Colour Technology, Paint Properties and Quality Control in Paint Industries

Colour science and technology - light spectrum, primary and complementary colours, colour mixing, dimensions of colour and colour systems, colour measurements, computer colour matching - colour coding system - general properties of paints, classification of paint properties - adhesion and cohesion properties, factors affecting adhesion wetting power, optical properties; colour, gloss, hiding, etc., physical, chemical and mechanical properties of paint films - factors affecting coating properties - rheological properties - Newtonian and non-Newtonian liquids, thixotropy, factors affecting viscosity, objectives of paint testing - quality control procedures, standard specifications and test methods - tests on liquid paints density, dispersion, viscosity and consistency, wet opacity and dry hiding, spreading capacity and spreading rim, wet and dry rim thickness, drying time, etc. - tests of dried coatings, colour and colour fastness, light fastness, gloss, flexibility, adhesion impact test, hardness mar resistance, abrasion resistance water and moisture resistance; water vapour transmission, PAC and salt spray test resistance, resistance to chemicals and solvents, resistance to heat and fire, air permeability - evaluation of water based paints, biological effects on paint films. Analysis of paints and varnishes; volatile and nonvolatile matter pigment content, binder or solid vehicle content, water content, ash content, pigment binder and solvent analysis - ageing properties of coatings, weatherometery, natural outdoor durability test, accelerated outdoor weathering, artificial weathering tests, defects observed in paint film on exposure.

TEXTBOOKS

1. *Australian OCCA, 'Surface Coating Technology Volume 1', Chapman and Hall, 1974.*
2. *W. M. Morgan, 'Outline of Paint Technology', John Wiley Sons, 1990.*

REFERENCES

1. *L. S. Pratt, 'Physics & Chemistry of Organic Pigments', Wiley, 1947.*
2. *H.Y. Payne, 'Organic Coating Technology Vol, 1 & 11', John Wiley & Sons, 1954.*

22CHY338 Forensic Science 3 0 0 3

Evaluation Pattern:

Assessment	**Internal**	**External**
Periodical 1 (P1)	15	
Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	
End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1 Introduction

Origin of forensic science, need for forensic science, trace and contact evidence, marks and impression, examination of documents, blood stain analysis, microscope in analysis, explosives, chemical analysis of explosives, forensic laboratories and courses in India.

Unit 2 Narcotics

Narcotics, classification of drugs, specific drugs- Psychotropic drugs, chemical screening of drugs, chemical extraction and sample preparation, chemical identification of drugs using analytical methods.

Unit 3 Fingerprinting and Firearm Analysis

History of fingerprinting, principles of fingerprinting, constituents of latent finger marks, fingerprint detection, chemical methods of detection, firearm examination, chemical analysis of firearm, analysis of gunshot residue.

Unit 4 Toxicology

Introduction to Toxicology, alcohol and human body, testing of blood alcohol concentration, toxins & biological poisons, measuring toxicity as LD50, sample and analysis, inorganic poisons, nerve agents, radioactive toxins, pharmacokinetics and toxicokinetics, tests for toxins, reported case studies.

Unit 5 Post-mortem Toxicology

Introduction, tissue and fluid specimens, specimen collection and storage, extraction procedure, analytical techniques, interpretation, case studies

REFERENCE

1. *Lawrence Kobilinsky, Forensic Chemistry Handbook, John Wiley & Sons, New Jersey, 2012*
2. *David E. Newton, Forensic Chemistry, Facts On File, Inc, New York, 2007*
3. *Jay A. Siegel, Forensic Chemistry fundamentals and applications, Wiley Balckwell.*
4. *Suzanne Bell, Drugs, Poisons, and Chemistry, Facts On File, Inc. New York, 2009.*

22CHY501 Advanced Physical Chemistry I 3 0 0 3

Quantum Chemistry

Evaluation Pattern:

Assessment	Internal	External
Periodical 1 (P1)	15	
Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	
End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1 Quantum Chemistry - Introduction

Origin of quantum mechanics, de Broglie relationship, the uncertainty principle (no derivation); Postulates of quantum mechanics: postulate I – wave functions, postulate II- Operators in quantum mechanics, operator algebra, postulate-III – eigen values, eigen value equations, postulate IV – expectation value, postulate V – time dependent and time independent Schrodinger equation

Unit 2 Applying Schrodinger Equation to Various General Systems

Translational motion of a quantum entity (particle in one dimensional box and three dimensional box); vibrational motion (harmonic oscillator); rotational motion (rigid rotator, particle on a ring and particle on

a sphere); angular momentum.

Unit 3 Atomic Structure and Chemical Bonding

Hydrogen and hydrogen-like atoms; multi electron systems- variation methods, perturbation methods, application to the ground state of helium atom, SCF method, the exclusion principle

Chemical bonding: hydrogen molecule ion and hydrogen molecule - molecular orbital and valence bond theory, homo and hetero nuclear diatomic molecules from VB and MO theory, the concept of directed valences and hybridization; quantum mechanics in band theory of metallic solids

Unit 4 Electronic Structure of Polyatomic Systems: Computational Quantum Chemistry

Semi empirical and ab-initio methods; QM approximations, Details of HMO and EHMO and its application to chemical bonding in unsaturated molecules (ethylene, 1,3butadiene etc); details of SCF procedure, Hartree and Hartree Fock methods (up to ground and excited states of hydrogen molecule); the basis sets, STOs and GTOs, nomenclature of basis sets, basis set errors, introductory ideas on DFT.

Unit 5 Molecular Properties: Computational Quantum Chemistry

Calculations of molecular properties like atomic charges, dipole moments, electronic distributions, vibration frequencies, NMR chemical shift etc using Gaussian program, specification of molecular geometry using cartesian coordinates and internal coordinates, Z-matrix, Z-matrix of some simple molecules, structure of a Gaussian input file

TEXTBOOKS

1. *Ira N. Levin, 'Quantum Chemistry', 6th Edition, Prentice-Hall, 2008*
2. *Peter Atkins, Ronald Friedman, 'Molecular Quantum Mechanics', 4th edition, Oxford university press*
3. *R K Prasad, 'Quantum Chemistry', New Age International (P) LTD publishers*

REFERENCES

1. *Andrew R Leech,'Molecular Modeling – Principles and Applications', 2nd Edition, Pearson Education.*
2. *Donald A. McQuarrie, 'Quantum Chemistry', Viva Books 2016.*

22CHY506 Advanced Inorganic Chemistry I 3 1 0 4

Evaluation Pattern:

Assessment	Internal	External
Periodical 1 (P1)	15	
Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	
End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1 Nuclear Chemistry

Nuclear structure, mass and charge, mass defect, binding energy, stability rules, magic numbers, nuclear quantum numbers, nuclear parity and statistics, models of nucleus, shell model, liquid drop model, semi empirical mass equation, equations of radioactive decay and growth, half-life, average life determination of half-lives, nuclear reactions, energetics of nuclear reactions, types of nuclear reactions, spontaneous and induced fission, neutron capture cross sections - critical size principle and working of nuclear reactor. Numerical problems relevant to each session.

Unit 2 Radiation Chemistry

Radioactive elements, decay kinetics, parent-daughter decay relationships, radioactive equilibrium-transient and secular equilibrium, alpha and beta decay, gamma emission, Radiochemical methods-measurement of radioactivity, measurement of radiations - ionization chamber, proportional counter, the Geiger counter, scintillation counter, semiconductor detectors. Applications of nuclear and radiation chemistry, isotope dilution analysis - activation analysis, radioactive tracers, radiometric titrations, radiation dosimetry, hydrated electron.

Unit 3 Inorganic Materials I

Alkali and alkaline earth metals, their compounds, crown ethers and cryptands as complexing agents for alkali metal ions, Be and Mg compounds, boron cage compounds, boron hydrides, structure and bonding, 3-centre-2-electron bonds, styx numbers, the importance of icosahedral frame work of boron atoms in boron chemistry, closo, nido and arachno structure, carboranes, metallocene carboranes, applications of boron clusters, B-N compounds, interstitial compounds, metal carbides, nitrides and hydrides, fullerenes, functionalized fullerenes, C-nanotubes .

Unit 4 Inorganic Materials II

Inorganic chains and polymers, rings, cages, and clusters, sulphur-nitrogen compounds, polymeric sulphur nitride, isopoly anions, heteropoly anions, Keggin and Dawson polyoxometallates, borazines, metal clusters, nature of Si-Si bonds, silicates, silicates with zero-, one-, two- and three-dimensional structures, structure of elemental P, phosphonitrilic compounds, polymers with P-N bonds, interhalogen and pseudo halogens, intercalation chemistry, intercalation in layered materials like graphite, xenon fluorides & other xenon compounds.

Unit 5 Chemistry of f-Block Elements

The lanthanides and actinides, stable oxidation states, the lanthanide and actinide contractions, the f-orbitals, spectral and magnetic properties - comparison with inner transition and transition metals, separation of lanthanides, use of lanthanide compounds as shift reagents, photo-emission of lanthanide compounds, organometallic compounds of lanthanides and actinides and their structural features, reactions of lanthanide and actinide compounds, mineral sands of south west India - Ilmenite, monazite, etc.

TEXTBOOKS

1. *H J Arnikar, Essentials of Nuclear Chemistry, 4th revised edition, New Age International (P) Limited publishers, 2015.*
2. *H J Arnikar, Nuclear Chemistry through Problems, New Age International Publishers.*
3. *J. Huheey, Inorganic Chemistry: Principles of Structure and Reactivity, 4th edition, 2006.*
4. *F.A. Cotton, Advanced Inorganic Chemistry, Wiley; 6th Edition (22 April 1999)*
5. *J.D. Lee Concise Inorganic Chemistry, Oxford University Press, 5th edition, 2008*

REFERENCES

1. *Gregory R. Choppin, Jan-Olov Liljenzin and Jan Rydberg, Radiochemistry and Nuclear Chemistry (Third Edition), Elsevier, 2002*
2. *Walter D. Loveland, David J. Morrissey, Glenn T. Seaborg, Modern nuclear chemistry, A JOHN WILEY & SONS, INC., PUBLICATION, 2017.*
3. *Shriver and Atkins' Inorganic Chemistry, Oxford; 5th edition, 2009*

22CHY507 Advanced Organic Chemistry I 3 0 0 3

Evaluation Pattern:

Assessment	Internal	External
Periodical 1 (P1)	15	
Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	
End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1 Concepts in Organic Reactions

Nucleophilic Substitution: SN_1, SN_2, and borderline (ion pair), SNi, SET mechanisms, neighbouring group participation, ambident nucleophiles and substrates. Aromatic nucleophilic substitution: SN_{Ar}, SN_1, benzyne and SRN_1 mechanisms. Effect of substrate structure, leaving group and attacking nucleophile on reactivity. SE_2 and SE_i, SE_1, substitution accompanied by double bond shift. Aromatic electrophilic substitution: arenium mechanism, free radical reactions: radical addition. Effect of substrate (aliphatic, aromatic, bridgehead), nature of the radical and solvent on reactivity. Addition reactions: mechanism of electrophilic, nucleophilic and radical addition. Elimination reactions: mechanism of elimination reactions E_2, E_1, E_{1CB}, steric effect. Catalysis by acids and bases and nucleophiles with examples from acetal, cyanohydrin and

ester formation and hydrolysis reactions - AAC_2, AAC_1, AAL_1, BAC_2 and BAL_1 mechanisms. Solvent effect - bulk and specific solvent effects. Introduction to carbon acids – pKa of weak acids, kinetic and thermodynamic acidity. Hard and soft acids and bases – HSAB principle and its applications.

Unit 2 Physical Organic Chemistry

Group electronegativity, molecular quadruple moment, polarizability, QMOT of methyl group, flash diagram of methyl group, internal strain and relative stability of molecules, bond dissociation energy - prediction of exothermicity and endothermicity, potential functions and surfaces - energy surfaces, reaction coordinate diagrams, transition state theory (TST) - mathematical formulations of transition state, Boltzmann distributions and temperature dependence. Experimental determinations of activation parameters and Arrhenius parameters, examples of activation parameters and their interpretations, postulates and principles related to kinetic analysis, The Hammond postulate - reactivity vs. selectivity principle, the Curtin-Hammett principle, microscopic reversibility, kinetic vs. thermodynamic control , steady state kinetics, applications of SSK, saturation kinetics, prior rapid equilibria, fast kinetic techniques-flow technique, flash photolysis, pulse radiolysis and relaxation methods. More O'Ferrall-Jencks plot methods used for determining kinetics, calculating rate constants.

Unit 3 Theoretical Concepts in Organic Reaction Mechanism: Experiments related to thermodynamics and kinetic isotope effects, primary kinetic isotope effects, reaction coordinate diagrams and isotope effects, primary kinetic isotope effects for linear transition states and non-linear transition states, the origin of secondary kinetic isotope effects, isotopic perturbation of equilibrium applications to carbocations, tunnelling, solvent isotope effects, heavy atom isotope effects, substituent effects, Hammett plots - sigma and rho values, predicting mechanisms. Linear free energy relationship, Taft equation - Taft parameters, solvent effects- Grunwald - Winstein plots, deviations from linearity, separating resonance from induction, steric and polar effects - Taft parameters, Schleyer - nucleophilicity and nucleofugality - Swain-Scott parameters, acid-base related effects - βnuc, βic, experiments for studying mechanisms - cross-over experiments, stereochemical analysis, isotope scrambling, transient spectroscopy, enzyme catalysis - Michaels Menten kinetics - meaning of K_m, Turnover number, line weaver bruk plot, perfect enzymes.

Unit 4 Optical Isomerism

Introduction to molecular symmetry and chirality: examples from common objects to molecules. Axis, plane, centre, alternating axis of symmetry. Centre of chirality: molecules with C, N, S based chiral centres, absolute configuration, enantiomers, racemic modifications, R* and S* nomenclature using Cahn-Ingold-

Prelog rules, molecules with a chiral centre and C_n, molecules with more than one centre of chirality, definition of diastereoisomers, relative configuration of diastereomers. Stereoselectivity: Classification, terminology, principle of stereoselectivity, examples of diastereoselectivity using Cram, Cram-Chelate, Felkin-Ahn, anti-Felkin, Houk models, Cieplak and cation coordination models, and Zimmerman-Traxler transition states, enantioselectivity. Desymmetrization and kinetic resolution, methods of determination of absolute configuration. Auwers-Skita rule, NOE effect, anomeric effect, constitutionally symmetrical and unsymmetrical chiral molecules, axial, planar, and helical chirality with examples, stereochemistry and absolute configuration of allenes, biphenyls and binaphthyls, ansa and cyclophanic compounds, spiranes, helicenes, annulenes, atropisomerism. Topicity and prostereoisomerism, exo-cyclic alkylidene cycloalkanes. Topicity of ligands and faces as well as their nomenclature. NMR distinction of enantiotopic/diastereotopic ligands. Stereoisomerism: definition based on symmetry and energy criteria, configuration and conformational stereoisomers, prochiral centre.

Unit 5 Conformational Analysis

Factors affecting conformational stability of molecules. Conformational analysis of acyclic and cyclic systems: butane, cyclohexane and its derivatives, decalins and other ring systems, adamantane, congressane, sucrose and lactose. Fused and bridged bicyclic systems. Conformation analyses of heterocycles. and reactivity of elimination (dehalogenation, dehydrohalogenation, semipinacolic deamination and pyrolytic elimination - Saytzeff and Hofmann eliminations, substitution and oxidation of secondary alcohols. Stereochemistry in cycloaddition reaction. Molecular dissymmetry and chiroptical properties - ORD, CD, octant rule (cyclohexanones), axial halo ketone rule, conformation and reactivity - classical and nonclassical carbocations, stereoselective and stereospecific reactions. Double stereo differentiation.

TEXT BOOKS

1. *Michael B Smith, "March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure", 7th edition, Wiley (2015).*

2. *Francis A. Carey and Richard J. Sundberg, "Advanced Organic Chemistry - Part A: Structure and Mechanisms", 5th Edition, Springer, 2008*
3. *P. S. Kalsi, "Stereochemistry, Conformation and Mechanism", New Age Publications, 2008*
4. *R. Bruckner, Advanced Organic Chemistry: Reaction Mechanisms, Academic Press, 2002.*
5. *F.A. Carey, R.A. Sundberg, Advanced Organic Chemistry, Part A: Structure and Mechanisms, 5th Edn., Springer, 2007.*
6. *J. Clayden, N. Greeves, S. Warren, P. Wothers, Organic Chemistry, Oxford University Press, 2004.*
7. *T.H. Lowry, K.S. Richardson, Mechanism and Theory in Organic Chemistry, 2nd Edn., Harper & Row, 1981.*
8. *N.S. Isaacs, Physical Organic Chemistry, ELBS/Longman, 1987.*

REFERENCES

1. *E. L. Eliel and S. H. Wilen, "Stereochemistry in Organic Compounds", John Wiley, 2008.*
2. *D. Nasipuri, "Stereochemistry of Organic Compounds - Principles and Applications", 4th Revised Edition, New Academic Science, 2012.*
3. *Peter Sykes, "A Guidebook to Mechanism in Organic Chemistry", Pearson Education; 6th edition, 2003.*

22CHY512 Molecular Spectroscopy 3 1 0 4

Evaluation Pattern:

Assessment	Internal	External
Periodical 1 (P1)	15	
Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	
End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1 Rotational and Vibrational Spectroscopy

Introduction to spectroscopy, rotation spectra - diatomic and polyatomic molecules, selection rules, intensities of spectral lines, stark effect, instrumentation of micro wave spectroscopy, applications and structural determinations, vibration spectra of diatomic molecules, harmonic and anharmonic vibrations, diatomic vibrating rotor, selection rule, breakdown of Born Oppenheimer approximation, rotational character of vibration spectra, different modes of vibrations, vibration-rotation spectra, Fermi resonance, vibration spectra of polyatomic molecules, IR spectra of organic and inorganic compounds, phase, temperature and solvent dependence, FTIR technique, instrumentation, Raman spectra (including the use of laser) - theory, relation with IR spectroscopy, mutual exclusion principle, resonance Raman, stimulated hyper and inverse Raman effects, instrumentation and applications of Raman spectroscopy.

Unit 2 UV-Visible and Fluorescence Spectroscopy

Electronic spectra of atoms - single and multi-electron systems, j-j and L-S coupling, electronic spectra of diatomic and polyatomic molecules, its relation to electronic arrangement and symmetry of molecules, application of group theory in electronic spectra, selection rules, nature of electronic excitation, principles of absorption spectroscopy, Beer-Lambert law, presentation of spectra, chromophores, forbidden transition, different types of electronic transitions, p-p*, n-p* etc transitions, nature of transitions in carbonyl compounds, the effect of conjugation, effect of conjugation on alkenes, HOMOs and LUMOs, Woodward-Fieser rules for dienes, spectra of carbonyl compounds, enones, Woodward rule for enones, spectra of aromatic compounds, effect of substituents, structural information from electronic spectra, excited states of molecules, fluorescence and phosphorescence, Jablonski diagram in detail, lifetime of excited states, quantum yields, photosensitization, application of UV-Visible and Fluorescence spectroscopy for structural elucidation of organic compounds and coordination complexes, diffuse reflectance spectra.

Unit 3 NMR Spectroscopy

Nuclear magnetic resonance phenomenon - theory, relaxation effects, NMR uses active nuclei, Fourier Transformation in NMR, measurement of relaxation time, chemical shift, magnetic anisotropic effect, multiplets in NMR, spin-spin splitting, n + 1 rule, Pascal's triangle, tree-diagram, spin-spin splitting constant, J, ^{2}J and ^{3}J and long-range coupling, measurement of J, Karplus relationship, first and second order spectra, AX, AB, AX_2, AX_3, A_2X_3, AMX type spectra, double resonance and spin tickling, chemical shift reagents, spectra in higher fields, spectra of conformational isomers, homotopic, enantiotopic and diastereotopic systems, C^{13} spectra, factors related to ^{13}C spectra, ^{1}H coupled ^{13}C spectra, ^{1}H decoupled ^{13}C spectra, chemical shift values, nuclear Overhauser effect (NOE), cross-polarization, off-resonance resonance decoupling, application of ^{1}H and ^{13}C NMR spectroscopy for the structural elucidation of organic compounds, ^{11}B, ^{15}N, ^{19}F and ^{31}P NMR spectra, spectra of paramagnetic complexes, magnetic susceptibility, contact shift, fluxional molecules and their studies using NMR, solid state NMR. Homonuclear and Heteronuclear correlation NMR.

Unit 4 ESR, NQR and Mossbauer Spectroscopy

ESR spectroscopy - theory, hyperfine and superfine splitting, ESR active simple organic systems, ESR of inorganic systems like Cu^{2+} and VO^{2+} complexes, 'g' markers like DPPH and TCNE, evaluation of spin Hamiltonian like A, $g_{||}$, g-, covalency factor in Cu^{2+} complexes, analysis of ESR spectra of VO^{2+} complexes, NQR spectroscopy - theory, relationship between electric field gradient and molecular structure, quadrupole coupling constant and structural information of compounds, Mossbauer spectroscopy, principle, Doppler effect, isomer shift, Zeeman splitting, quadrupole splitting, application of Mossbauer spectroscopy for studying Fe and Sn compounds and phase transformation, application of ESR spectroscopy.

Unit 5 Mass Spectrometry and PES

Mass spectroscopy, base peak and molecular ion peak, isotope ratio data, fragmentation patterns of alkanes, alkenes, alkynes, aromatic hydrocarbons, alcohols, phenols, aldehydes, ketones, esters, carboxylic acids, amines, methods of desorption and ionization (EI, CI, LD, MALDI, PD, FAB, SIMS), MS/MS and determination of molecular formula, metastable ions and their significance, study of fragmentation pattern, application of MS in structural elucidation and other frontiers of science, application of MS for quantitative analysis, photoelectron spectroscopy (PES), principle, application of PES. Structure determination using IR, UV-visible, NMR, MS and ESR spectral techniques.

TEXTBOOKS

1. *Colin N. Banwell and Elaine M. McCash, 'Fundamentals of Molecular Spectroscopy', 4th Edition, Tata McGraw Hill, 2007.*
2. *W. Kemp, Organic Spectroscopy, 3rd Edition, McMillan International Higher Education*
3. *D. L. Pavia, G. M. Lampman, G. A. Kriz, and J. R. Vyvyan, Introduction to Spectroscopy, 5th Edition, Brooks-Cole, 2009*
4. *G. M. Barrow, 'Introduction to Molecular Spectroscopy', McGraw Hill, 1962.*
5. *R. M. Silverstein, F. X. Webster, D.J. Kiemle, Spectroscopic identification of organic molecules, 7th Edition, John Wiley*
6. P. S. Kalsi, Spectroscopy of Organic Compounds: New Age International Pvt Ltd 6th edition, 2006

REFERENCES

1. *Hollas, J.M., Modern Spectroscopy, John Wiley & Sons, Fourth Edition, 2004*
2. *J. Keeler, Understanding NMR spectroscopy, Wiley, 2009*
3. *D. A. Skoog, F. J. Holler and S. R. Crouch, 'Principles of Instrumental Analysis', 6th Edition, Thomson Brooks/Cole, 2007.*
4. *W. Kemp, NMR in Chemistry, McMillan, 1988*
5. *J. E. Wertz and J. R. Bolton Electron Spin Resonance, Springer Science*

Evaluation Pattern:

Assessment	Internal	External
Periodical 1 (P1)	15	
Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	
End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1 Introduction to Molecular Point Groups

Definition of a mathematical group, symmetry in molecules, elements of symmetry, matrix representation of symmetry operations, molecular point groups, abelian group, cyclic group, symmetry operations as group elements, similarity transformation and classes, group multiplication table, symmetry classification of molecules into point groups (Schoenflies symbol)

Unit 2 Construction and Interpretation of Character Tables

Reducible and irreducible representations, great orthogonality theorem and its consequences, character tables, reduction formula, construction of character tables for point groups with order ≤6, interpretation of character tables.

Unit 3 Applications of Group Theory - I (Vibrational and Electronic Spectroscopy)

Infrared and Raman activity of molecular vibrations in H_2O, N_2F_2, BF_3, AB_4 type molecules (Td and D_4h) and AB_6 type (Oh) of molecules; selection rules; electronic structure of free atoms and ions, splitting of terms in a chemical environment, construction of energy level diagrams, estimations of orbital energies, selection rules and polarizations, double groups, a brief idea on electronic spectra of transition metal complexes – selection rules, Orgel diagrams, Tanabe Sugano diagrams.

Unit 4 Applications of Group Theory (Chemical Bonding - Hybridization and Molecular Orbital Formation)

Group theory to explain hybridization - wave functions as bases for irreducible representations, construction of hybrid orbitals for AB_3 (planar), AB_4 (Td), AB_5 (D_{3h}) and AB_6 (O_h) type of molecules, symmetry adapted linear combinations, projection operators, application of projection operators to pi-bonding in ethylene, cyclopropenyl systems and benzene, application of symmetry to predict polar and chiral compounds;

Unit 5 Symmetry in Solid State

Symmetry elements and operations in solid state – proper axis of rotation, mirror planes of symmetry, roto-reflection and roto-inversion axes of symmetry, screw axes of symmetry, glide planes; a brief introduction to the crystallographic point groups and space groups

TEXTBOOKS

1. *F. Albert Cotton, 'Chemical Applications of Group Theory', 3rd Edition, John Wiley, 1990.*
2. *A Salahuddin Kunju, G Krishnan; 'Group theory and its application in chemistry', second edition, PHI Learning private limited-2015*

REFERENCES

1. *Robert L Carter, 'Molecular symmetry and Group theory', John Wiley & Sons, Inc.*
2. *V. Ramakrishnan and M.S. Gopinathan, 'Group Theory in Chemistry', 2nd reprint edition, Vishal Publications, 1996.*
3. *P.H. Walton, "Beginning Group Theory for Chemistry", Oxford University Press Inc., New York, 1998.*

22CHY581 Inorganic Semi-Micro Qualitative Analysis Lab 0 0 5 2

Semimicro Analysis of Mixtures

The mixture will include 4 cations including two common (eg. Cations of metals like Cu, Mn, Zn, Ni, Ca, Ba, Mg etc.) and two less common cations (eg. Cations of metals like Ti, Zr, V, W, Li, Ce, Th etc.).

(The student has to successfully analyze a minimum of 10 mixtures).

TEXTBOOKS

1. *A.I. Vogel, 'A text book of Qualitative Analyses', 4th edition, Longmans publications, 1985.*
2. *V.V. Ramanujam, 'Inorganic Semi-Micro Qualitative Analysis', 3rd edition, The National Publishing Company, 1974.*

22CHY582 Organic Quantitative Analysis Lab 0 0 5 2

A. Estimations:

Estimation of (i) equivalent weight of an acid, (ii) glucose (iii) phenol (iv) acetone (v) acid value of an oil (vi) iodine value and sap value of an oil (vii) formaldehyde (viii) aniline (ix) ester

Estimation of the following drugs: Aspirin (titrimetry), ibuprofen (titrimetry), analgin (titrimetry), ascorbic acid {titrimetry (Iodometry and Cerimetry), colorimetry}, Riboflavin (colorimetry), Zn ions in Bacitracin Zinc, Ca^{+2} ions in calcium gluconate injection (complexometry), diazepam (UV-Visible Spectrophotometer).

B. Preparations of Organic Compounds

Double stage preparations:

(a) m-nitro benzoic acid from ethyl benzoate (b) p-bromobenzanilide from aniline (c) p-nitro acetanilide from aniline

Single stage preparations:

(a) Benzimidazole (b) Benzophenone oxime (c) Dibenzilidene acetone (chalcone) (d) Benzanilide (e) Benzalacetophenone (f) Acetanilide (g) Acetyl salicylic acid (aspirin)

Name Reactions:

(a) Benzil-Benzilic acid rearrangement
(b) Cannizaro reaction
(c) Claisen condensation

For all preparations

1. TLC to be done and R_f values of each compound to be reported
2. Melting point of pure compounds to be found
3. A small portion should be recrystallized from suitable solvent
4. Purified products to be displayed
5. Mechanisms for each preparation should be suggested

Identification of unknown organic compounds from their IR, UV,1H NMR and Mass Spectral data: Analysis of recorded spectra of compounds belonging to i) alkynes, ii) alcohols and phenols iii) aldehydes and ketones iv) carboxylic acids, v) esters, vi) acid amides and vii) primary and secondary amines.

REFERENCES

1. *P.W.G. Smith, A.J. Hannaford, B.S. Furnis and A.R. Tatchell, "Vogel's Textbook of Practical Organic Chemistry", ELBS/Longman, 1989.*
2. *Ralph L. Shriner, Christine K. F. Hermann, Terence C. Morrill, David Y. Curtin, Reynold C. Fuson, 'Systematic Identification of Organic Compounds', John Wiley & Sons, 2003.*
3. *Mann and Saunders, 'Practical Organic Chemistry', Pearson edition, 2009*

22CHY511 Advanced Physical Chemistry III 3 1 0 4

(Chemical Thermodynamics and Equilibrium)

Evaluation Pattern:

Assessment	Internal	External
Periodical 1 (P1)	15	
Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	
End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1 Chemical Thermodynamics

First and second laws of thermodynamics, thermodynamic functions, heat capacity, thermochemistry, need for second law of thermodynamics, entropy and free energy functions, calculation of changes in thermodynamic function for ideal and non-ideal gases in isothermal and adiabatic process, relation between thermodynamic functions - Maxwell relations, Joule Thomson effect, coefficient of thermal expansion and compressibility factor, applications of free energy function to physical and chemical changes, equilibrium in chemical reactions, third law of thermodynamics - need for third law, calculation of absolute entropy, unattainability of absolute zero, thermodynamic systems of variable composition - fugacity functions, partial molar quantities, thermodynamics of ideal solutions, real solutions and regular solutions, dilute solutions of nonelectrolytes, Henry's law, Raoult's law, Gibbs-Duhem equations, Gibbs-Duhem-Margules equations, and activity and standard states of non-electrolytes.

Unit 2 Irreversible Thermodynamics

Examples for irreversible process, entropy production, non-equilibrium, steady state and near equilibrium conditions, linear relation, phenomenological coefficients, Onsager reciprocal relations, one component systems with heat and matter transport, application of irreversible thermodynamics to thermal diffusion, thermal osmosis etc., electro kinetic effects, the Glansdorf - Pregogine equation.

Unit 3 Statistical Thermodynamics

Statistical concept, probability and thermodynamic states, entropy and probability, canonical ensemble, Maxwell-Boltzmann, Fermi-Dirac and Bose-Einstein Statistics, electron gas concept, Bose-Einstein condensation, relation among MB, FD & BE Statistics, partition function, partition function for free linear motion, free motion in a shared space, linear harmonic vibration, translational, rotational and vibrational partition function, molecular partition functions, partition functions and thermodynamic properties, calculation of equilibrium constant, heat capacity of gases, mono atomic solids, Einstein's and Deby's theory.

Unit 4 Equilibrium

Gibb's free energy, direction of spontaneous change of a reaction, chemical potential, chemical potential and equilibrium, ΔG in terms of K, equilibrium constants – real gases and real reactions, equilibrium respond to catalyst, temperature, pressure and $_P$H, application of ΔG and K – extraction of metals from their oxides, Ellingham diagram, and thermodynamics of ATP & respiration, biological energy conversion.

Unit 5 Phase Equilibrium

Gibb's Phase rule, one component system, two component systems, vapour pressure diagrams and their interpretation, lever rule, temperature-composition diagrams, liquid-liquid phase diagrams, distillation of partially miscible liquids, azeotropes, liquid-solid phase diagrams, phase diagram for the system Na/K/Na_2K, phase diagram - steel, alloys, Fe-C system, zone refining, three component system, triangular coordinates, three component system – partially miscible liquids - $H_2O/CHCl_3/CH_3COOH$, phase diagram - $NH_4Cl/(NH_4)_2SO_4/H_2O$

TEXTBOOKS

1. *Robert J. Silbey, Robert A. Alberty, Moungi G. Bawendi, Physical Chemistry 4th Edition, Wiley, 2004*
2. *Samuel H. Maron, Carl F. Prutton Principles of Physical Chemistry, The Macmillan Company; 4th edition (1970)*
3. *Samuel Glasstone, 'Thermodynamics for Chemists', Lightning Source Incorporated, 2007.*

REFERENCES

1. *Francis Weston Sears and Gerhard L. Salinger, 'Thermodynamics, kinetic theory and statistical thermodynamics' 3rd edition, Addison-Wesley Publications, 1975.*
2. *Prigogine, 'Introduction to Thermodynamic Irreversible Processes', Interscience Publishers, 3rd edition, 1968.*
3. *R.P. Rastogi and R.R. Misra, 'An Introduction to Chemical Thermodynamics', 6th Revised edition, Vikas Publishing House Pvt. Ltd., 2006.*
4. *F.W. Sears, 'Introductions to Thermodynamics, Kinetic Theory of Gases and Statistical Mechanics', Addison Wesley Pub., Cambridge, 1972.*

22CHY516 Advanced Organic Chemistry II 3 1 0 4

Evaluation Pattern:

Assessment	Internal	External
Periodical 1 (P1)	15	
Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	
End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1 Organic Photochemistry

Photochemistry: Introduction – photochemical verses thermal reactions. Photochemical energy - photochemical excitation of the molecule, electronic transitions, photolytic cleavage. Reactions involving olefin bond, cis-trans isomerisation, valence bond tautomerisations. Reaction proceeding through bond dissociation - Norrish reactions of acyclic ketones, Fries, dienone – phenol, Favorski and di – pi methane rearrangement, Barton reaction, photofragmentation, photoaddition, photosubstitutions, cycloadditions, Paterno Buchi reaction, Lumiketone rearrangement, mechanism of 1,3 acyl shift, photochemical oxidations and reduction, singlet oxygen and chemiluminescence. Dye-sensitized photooxygenations, photochromism, photochemistry of polymers, photoinduced electron transfer (PET) reactions, photochemistry of vision.

Unit 2 Pericyclic Reactions: Energy considerations of thermal and photochemical reactions, concept of ionic, concerted, synchronous and non–synchronous pathways. Classification of pericyclic reactions - electrocyclic, cycloadditions and, sigmatropic reactions (cheletropic and group transfer reactions). Theory of pericyclic reactions – symmetric properties of MO, Con and Dis rotator modes, correlation diagrams,Woodward- Hoffmann rules. Analysis of pericyclic reactions using FMO and related methods. Stereochemistry and regiochemistry of pericyclic reactions, exo - endo selectivity in Diels – Alderreactions, Cope and Claisen rearrangement, Baldwin rules for ring closure, applications of pericyclic reactions to organic synthesis.

Unit 3 Chemistry of Reactive Intermediates

Chemistry of enolates, enamines. Kinetic and thermodynamic enolates - boron enolates in aldol and Michael reactions, alkylation and acylation of enolates. Name reactions of carbanions - Clasien, Dieckmann, Stobbe, Darzen, and acyloin condensation, Shapiro reaction and Julia – elimination. Chemistry of phosphorus and sulphur ylids - Wittig and related reactions, Petersons olefination. C-X bond formation (X = C, O, N) through the intermediary of carbocations - molecular rearrangements including Wagner-Meerwein, pinacol – pinacolone, semi- pinacol, dienone- phenol and benzylic acid rearrangement, Noyori annulations, Prins reactions. C-C bond formation involving carbocations - Oxymercuration, and halolactonizations. Generation, structure and reactivity of carbenes and nitrenes - Wolff rearrangement, Hofmann, Curtius, Lossen, Schmidt, and Beckmann rearrangements. Radicals: Generation of radical intermediates and its (a) addition to alkenes, alkynes (inter & intramolecular) for C-C bond formation and Baldwin's rules (b) fragmentation and rearrangements. Name reactions involving radical intermediates such as Barton deoxygenation and decarboxylation, McMurry coupling, etc.

Unit 4 Asymmetric Synthesis.

Asymmetry in nature, chiral pool, asymmetric induction, enantiomeric and diastereomeric excess, chiral reagents and chiral catalysts, chiral auxiliaries, Evans chiral oxazolidones, Davis chiral sulphinimines, asymmetric hydrogenation with Rh and Ru complexes, Noyory's hydrogenation, enantioselective hydrogenation of ketones using borohydrides reagents, DKR - definition, principles and examples. Asymmetric oxidations - epoxidation of allylic alcohols with Ti complexes - Sharpless epoxidation, epoxidation of unfunctionalized alkenes- Jacobsen – Katzuki epoxidation, Shi epoxidation, Aggarwal epoxidation, Beller epoxidation, epoxidation using Ru and Fe complexes. Asymmetric amino hydroxylation, asymmetric aldol reaction, asymmetric Pauson - Khand reaction.

Unit 5 Modern Synthetic Methods and Reagents

Baylis - Hillman reaction, Henry reaction, Nef reaction, Kulinkovich reaction, Ritter reaction, Sakurai reaction, Tishchenko reaction, Brook rearrangement, Tebbe olefination, Metal mediated C-C and C-X coupling reactions - Heck, Stille, Suzuki, Suzuki - Miyamura, Negishi- Sonogashira reactions, Nozaki-Hiyama, Buch – Wald – Hartwig, Ullmann, and Glaser Coupling reactions. Wohl-Ziegler reaction. Reagents

such as NBS, DDQ and DDC. Gilman reagent. **Multicomponent reactions** - introduction to MCR, Passserini reaction, Ugi reaction, Biginelli reaction. Introduction to combinatorial chemistry and click chemistry and its applications. Phase transfer catalysis and its application in organic synthesis.

TEXT BOOKS

1. *Michael B Smith, "March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure", 7th edition, Wiley (2015).*
2. *Francis A. Carey and Richard J. Sundberg, "Advanced Organic Chemistry – Part A: Structure and Mechanisms", 5th Edition, Springer, 2008*
3. *Francis A. Carey and Richard J. Sundberg, "Advanced Organic Chemistry – Part B: Reactions and Synthesis", 5th Edition, Springer, 2008.*
4. *Singh S P and SM Mukherji, "Reaction Mechanism in Organic Chemistry", 2014*

REFERENCES

1. *Reinhard Bruckner, Advanced Organic Chemistry, Reaction Mechanisms, Elsevier, 2002*
2. *R.O.C. Norman and J.M. Coxon, "Principles of organic synthesis", CRC press, 2014*
3. *Ian Fleming, Frontier Orbitals and Organic Chemical Reactions 1st Edition, Wiley, 1991*

22CHY504 Advanced Inorganic Chemistry II 3 0 0 3

Coordination Chemistry

Evaluation Pattern:

Assessment	Internal	External
Periodical 1 (P1)	15	
Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	
End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1 Theories and Concepts on *d*-Block Coordination Compounds

Introduction - ligands, nomenclature of coordination compounds, coordination compounds of *d*-block ions with coordination numbers of 2, 3, 4, 5, 6, 7 and 8. Werner's coordination theory, Valence bond theory (VBT), Crystal field theory (CFT), CFSE, effects of CFSE on hydration energies and spinel groups (normal and inverse), types of ligands – spectrochemical series, spectral and magnetic properties (spin-only magnetic moments), nephelauxetic effect. Crystal field splitting patterns in complexes having Oh, Td, square planar, square pyramidal and trigonal pyramid geometries, factors affecting the magnitude of CFSE, various types of isomerism in coordination complexes, Jahn-Teller (JT) distortion, manifestation of JT on spectral properties. Molecular orbital theory (MOT), ligand field theory (LFT), molecular orbital energy level diagram for octahedral complexes without pi-bonding, metal-ligand pi-bonding, metal-metal multiple bonds, *d*-orbital based metal-metal σ, π and δ bonds in compounds like $[Re_2Cl_8]^{2-}$, $[Os_2Cl_8]^{2-}$, $Cr_2(CH_3COO)_4$ and R-Cr(I)-Cr(I)-R. Application of group theory to coordination compounds.

Unit 2 Reaction Mechanism

Complex equilibrium - formation constants, chelate and macrocyclic effects, factors affecting stability of complexes, methods of determination of stability constants, stability of complex ions in solutions, inert and labile complexes, mechanisms of ligand displacement and addition reactions in octahedral complexes and square planar complexes of platinum *cis*- and *trans*-effect, substitution reactions, mechanisms of substitution, kinetic consequences of reaction pathways, dissociation, interchange, association, dissociation, linear free energy relationships, conjugate base mechanism, stereochemistry of reactions (substitution in *trans*-complexes and substitution in *cis*-complexes), isomerisation of chelate rings, sigma-bonding and pi-bonding effects, oxidation-reduction reactions, inner and outer sphere electron transfer reactions, conditions for high and low oxidations numbers, reactions of coordinated ligands, hydrolysis of esters, amides and peptides, template reactions, electrophilic substitution, photochemical reactions of coordination compounds. Asymmetric synthesis catalysed by coordination compounds

Unit 3 Coordination Chemistry of Inner-Transition (*f*-block) Elements

f-block metal ions – oxidation states preferences, ligand preferences, coordination numbers and the geometry of the complexes, influence of lanthanide contraction and actinide contraction in their coordination behaviour, shapes of *f*-orbitals (4*f* and 5*f*), nature of bonding of *f*-orbitals with ligands, various types of coordination compounds of lanthanides and actinides, stereochemistry and reaction mechanism of *f*-block metal complexes.

Unit 4 Spectral Properties

Stabilization of unusual oxidation states, electronic spectra of transition metal complexes – colour wheel, Russell-Saunders coupling schemes, term symbols for various d^n ions, Orgel diagrams for d^n systems, ligand field parameters, *Dq*, Racah parameter *B* and nephelauxetic constant *b*, Tanabe-Sugano (TS) diagrams, evaluation of *Dq* and other parameters from electronic spectra of transition metal complexes using TS diagrams, charge-transfer transitions, MLCT and LMCT, selection rules and band intensities, Laporte- and spin- selection rules, symmetry, spin-orbit and vibronic coupling effects. Photochemistry of transition metal complexes like $[Ru(bipy)_3]^{2+}$, spectral behaviour of *f*-block coordination complexes, special features of their absorption and emission properties.

Unit 5 Magnetic Properties

Magnetic properties of coordination complexes - magnetic susceptibility, contribution of spin-orbit coupling on μ_{eff}, types of magnetic behaviour - para-, ferro-, anti-ferro- and ferri-magnetic systems, Curie law, Curie-Wise law, Guoy, Faraday and superconducting quantum interference device (SQUID) methods, Kotani plots, giant magnetoresistance (GMR), anisotropic magnetoresistance (AMR) effect, effects of temperature on magnetic behaviour, tunnelling magnetoresistance (TMR). Magnetism of coordination complexes by multinuclear homo- and heterometallic 3*d* systems (also with exclusive 4*d* and 5*d* metal ions), mixed 3*d*-4*f* systems, importance of 4*f*-metal ions for functional applications. Nanoscale magnetic systems based on coordination complexes - Single Molecule Magnets (SMMs), Single Ion Magnets (SIMs), Single Chain Magnets (SCMs), Spin-crossover complexes, magnetic refrigerants (magnetic coolers), magnetic storage systems - magnetic random-access memory (MRAM).

TEXTBOOKS

1. *F. A. Cotton and G. Wilkinson, 'Advanced Inorganic Chemistry', John Wiley & Sons, 2009.*
2. *James E. Huheey, Ellen A. Keiter and Richard L. Keiter, 'Inorganic Chemistry, Principles of Structure and Reactivity', Pearson education, 5th edition, 2009.*
3. *J. D. Lee, 'Concise Inorganic Chemistry', 5th edition, John Wiley & Sons, 2009.*
4. *P Atkins, T. Overton, J. Rourke, M. Weller, F. Armstrong, "Shriver & Atkins Inorganic chemistry", 4th Edition, Oxford University Press, 2008.*

REFERENCES:

1. *B. Douglas, D. McDaniel and J. Alexander "Concepts and Models in Inorganic Chemistry", 3rd Edition, Wiley, 2006.*
2. *Sushanta Dattagupta, 'A Paradigm Called Magnetism', World Scientific Publishing Co. Pvt. Ltd., 2008.*
3. *Helen C. Aspinall, 'Chemistry of the f-Block Elements', Volume 5 of Advanced chemistry texts, CRC Press, 2001.*
4. *N. N. Greenwood and A. Earnshaw, 'Chemistry of Elements', Butterworth and Heinemann, 2nd Edition, 2002*
5. *J. E. House, "Inorganic Chemistry", Academic Press, 2008.*
6. *T. Shinjo (Editor), 'Nanomagnetism and Spintronics', Elsevier, USA, 2nd Ed., 2014.*
7. *R. A. Layfield and M. Murugesu (Editors), 'Lanthanides and Actinides in Molecular Magnetism', Wiley-VCH Verlag& Co., 2015.*

22CHY517 Advanced Organic Chemistry III 3 0 0 3

Evaluation Pattern:

Assessment	Internal	External
Periodical 1 (P1)	15	
Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	
End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1 Heterocyclic compounds

Construction of heterocyclic ring systems, different approaches towards synthesis of 3, 4, 5 and 6 membered rings. Synthesis of 4 membered rings - oxetanes, cyclobutanes, ketene cycloadditions (inter and intra molecular), Pauson- Khand reaction, Bergman's cyclisation, Nazarov cyclisation, Mitsunobu reaction, cation – olefin cyclisation and radical olefin cyclisation, inter conversion of ring systems (contraction and expansion) - Demjenov reaction. Construction of macrocyclic rings - ring closing metathesis. Name reactions involving heterocyclic chemistry – Bartoli reaction, Corey – Chykovsky reaction, Paal – Knorr synthesis, Fisher –Indole synthesis, Bischler – Napieralski reaction, Pictet – Spengler synthesis, Chemical reactivity of 5 and 6 membered heterocycles - thiophene, Furan, Pyrrole, Imidazole, Pyrimidine, Indole.

Unit 2 Biosynthesis and Biomimetic Synthesis

Basic principles of biosynthesis of terpenes, steroids, alkaloids, carbohydrates and cyclodextrins. Preparation of alditols, proteins and nucleic acids. Biosynthesis of cholesterol, alpha-terpenol, morphine. Biomimetic synthesis of progesterone. Synthesis of prostaglandins, biosynthesis of fatty acids, steroids. Total synthesis of quinine, and heroin, Synthesis of abietic acid and shikimic acid.

Unit 3 Peptides

Synthesis of amino acids - Strecker and azlactone synthesis, reactions of amino acids, structure of proteins. Introduction to enzymes and coenzymes with special reference to the function of chymotrypsin, NAD, thiamine, pyridoxal. Solid phase synthesis – choice of resin, classification and reactions leading to peptide formation. Protection and deprotection in protein synthesis- common protecting groups used in peptide synthesis, protection groups used in solution phase and solid phase peptide synthesis (SPPS). Sequencing of proteins: reagents used to modify the α- amino group at the amino terminal, Edman degradation, mass spectrometry. Separation of amino acids by ion- exchange chromatography, nature of peptide bond – Ramachandran plot and CD spectroscopy. Biocatalysis with respect to conformations and structure and function relationship, vitamins as co enzymes. Metabolism: Overview of the following path ways – Glycolysis, TCA cycle.

Unit 4 Nucleic Acids

Transfer of genetic information: chemistry of nucleic acids, cyclic AMP, assembly of DNA, types of RNA, replication of DNA. Enzymology in eucaryotes and bacteria, translation, genetic code, protein biosynthesis, regulation of gene expression. Repair of DNA and recombinant DNA technology. A- and Z- forms of DNA

Unit 5 Green Synthesis

Principles of green chemistry: basic concepts, atom economy, twelve principles of green chemistry, principles of green organic synthesis. Green alternatives to organic synthesis: coenzyme catalyzed reactions, thiamine catalyzed benzoin condensation. Green alternatives of molecular rearrangements: pinacol-pinacolone and benzidine rearrangements. Electrophilic aromatic substitution reactions. Oxidation-reduction reactions. Clay catalyzed synthesis. Condensation reactions. Green photochemical reactions. Green Solvents: ionic liquids, supercritical CO_2, fluorous chemistry, general principles of microwave and ultrasound assisted organic synthesis

TEXT BOOKS

1. *I.L. Finar Organic Chemistry vol 2 (3rd.ed.) Longmans Green & Co. 1964*
2. *Sujata V. Bhat, Bhimsen A. Nagasampagi, Meenakshi Sivakumar, Chemistry of Natural Products, Springer 2005*

REFERENCES

1. *K. C. Nicolaou, Eric J. Sorensen, Classics in Total synthesis, Wiley, 1996.*
2. *Ashutosh kar, Chemistry of Natural Products, (Volume I and II), CBS*
3. *Biomaterials –novel materials from biological sources D. Byrom - Stockton press*
4. *Hand Book of Biodegradable polymers Catia Bastioli, - Rapra Tech*
5. *Surface modification of biomaterials: Methods analysis and applications R Williams - University of Liverpool, UK*
6. *Biopolymers, R.M. Johnson, L.Y. Mwaikambo and N. Tucker, Publisher Rapra Technology, 2003.*
7. *Hand Book of Bioplastics & Biocomposites for Engineering Applications Srikanth Pillai*

Evaluation Pattern:

Assessment	Internal	External
Periodical 1 (P1)	15	
Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	
End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1 Concepts and Metal Carbonyls

History and overview on organometallic compounds. Classification and nomenclature – hapticity of fragments, 18-electron and 16-electron organometallic compounds. Structure prediction based on '18 electron rule'. Metal carbonyls – synthesis and bonding of metal carbonyls (based on MO theory), donor and acceptor properties of CO, different types of binding modes of CO, poly-nuclear carbonyls with and without bridging groups, metal-metal bonding in M-CO clusters, cluster valence electron (CVE) count, CVE based structure prediction. IR spectral features of metal carbonyls, activation of CO by bonding with metal ions.

Unit 2 Types of Organometallic Compounds

Metal phosphines compounds of transition metals, M-N_2 (metal dioxygen), M-O_2 (metal dioxygen), M-NO (metal nitrosyl) and M-CN (metal cyanide/isocyanide) complexes, bonding and structural features. Organometallic compounds with π-donor ligands like olefins, acetylenes and allyl moieties. Metal derivatives of cyclic π-donors (metallocenes, sandwich/half-sandwich compounds, bent metallocenes), metal-carbon σ-donors (metal carbenes – Fischer carbenes, Schrock carbenes and *N*-heterocyclic carbenes, metal polyenes, metal carbines, metal alkyl/aryl derivatives). Organometallic chemistry of lithium and magnesium, aluminium alkyls and all other main-group organometallics. Structural features and nature of bonding in above compounds.

Unit 3 Structure and Bonding

Fragment molecular orbitals (FMO) of various organic and inorganic moieties like CH_3, CH_2, CH, BH_2, BH, NH_2, NH. FMO's (π-orbitals) of C_3H_5, C_4H_4, C_4H_6, C_5H_5, C_6H_6, C_8H_8. Inorganic fragments ML_n with varying number of L's. Symmetry and shape of their FMO's. Isolobal concept, iso-electronic and isolobal relationships between various organic and inorganic (ML_n) fragments. Structure and bonding between various organic and inorganic fragments based on MO level diagrams – metal-olefins, ML_n - cyclobutadiene, ML_n-carbene, ML_n-carbyne, ML_n-cyclopentadienyl systems, compounds with metal-metal multiple bonds (metal-metal σ, π and δ bonds).

Unit 4 Stereochemistry and Reactions

Stereochemically non-rigid molecules, fluxional nature of organometallic compounds (including Li-C, Mg-C), characterization of non-rigidity of organometallic compounds by NMR spectroscopy. Difference in NMR spectra of fluxional organometallic compounds at high and low temperatures. Characterization techniques of organometallic compounds (by NMR – ^{1}H, ^{13}C and ^{31}P NMR spectroscopy, Dynamic NMR, Mass spectrometry). Reactions involving various organometallic compounds - oxidative addition reactions, reductive elimination reactions, migratory insertion reactions, 1,1-type and 1,2-type insertion reactions, elimination reactions, β-hydride elimination reactions. Conditions for organometallic compounds to exhibit above reactions, cyclo-metalation and ortho-metalation reactions, agnostic interactions.

Unit 5 Organometallic Catalysis

Alkene hydrogenation using Wilkinson's catalyst, water-gas shift reaction, Mosanto process, Cativa process. Reaction steps in the above catalytic processes. Hydro-formylation reactions, catalytic addition of molecular oxygen to alkenes (Wacker process), Ziegler-Natta polymerization of alkenes, Fischer-Tropsch process, olefin-metathesis (types of Grubbs catalysts and Hoveyda–Grubbs catalysts), oligomerization of alkynes, aluminium alkyls in polymerization of olefins. Palladium based reactions such as Heck, Stille, Suzuki, Sonogashira, Buchwald-Hartwig couplings; Tsuji-Trost C-C bond formations. Homogeneous vs. heterogeneous organometallic catalysis (principles, mechanism and their applications). Organometallics - in industry, in medicine, in agriculture and in environmental science.

TEXTBOOKS

1. *J.E. Huheey, R.A. Keiter, R.L. Keiter, 'Inorganic Chemistry-Principles of Structure and Reactivity', 4th Edn., Prentice Hall, 1997.*
2. *P. Atkins, T. Overton, J. Rourke, M. Weller, F. Armstrong,' Shriver and Atkins Inorganic Chemistry', 4th Edn., Oxford University Press, 2006.*
3. *F.A. Cotton, G. Wilkinson, C.A. Murillo, M. Bochmann, 'Advanced Inorganic Chemistry', 6th Edn., Wiley-Interscience, 1999.*
4. *Anil Elias, Gupta B.D., "Basic Organometallic Chemistry", Universities Press; 2nd Edition 2013*
5. *J.D. Atwood, 'Inorganic and Organometallic Reaction Mechanism', 2nd Edition. Wiley-*

REFERENCES

1. *R. H. Crabtree, 'Organometallic Chemistry of the Transition Metals', John Wiley & Sons, 6th Ed.*
2. *VCH, 1997.*
3. *J. Tsuji, 'Transition metal reagents and catalyst innovations in organic synthesis', John-Wiley- & Sons, Ltd, New York, 2000*
4. *B.E. Douglas, D.H. McDaniel, J. J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn., Wiley-India, 2007.*
5. *M. Bochmann, Orgaonometallics: Complexes with Transition Metal-Carbon Sigma Bonds, Oxford University Press, 1994.*
6. *J. P. Collman, R G Finke and J R Norton "Principles and Applications of Organo-transition metal Chemistry" University Science Books, 1987.*
7. *W.K. Li, G.D. Zhou, T. Mak, Advanced Structural Inorganic Chemistry, Oxford University Press, 2008.*
8. *K. C. Nicolaou, 'Classics in Total Synthesis', Vols I-III, Wiley-VCH, 1996; 2003; 2011*
9. *Louis S. Hegedus and Bjorn C. G. Soderberg, Transition Metals in the Synthesis of Complex Organic Molecules,*

22CHY583 Advanced Physical Chemistry Lab 0 0 5 2

1. Construction of phase diagram for three component system.
2. Determination of equilibrium constant of the reaction, $KI + I_2 = KI_3$ by partition method.
3. Determination of molecular weight of poly vinyl alcohol by viscosity method
4. Determination of energy of activation of acidic hydrolysis of methyl acetate.
5. Kinetic study of the second order reaction between potassium persulphate and potassium iodide.
6. Determination of equivalent conductance at infinite dilution of weak electrolytes.
7. Determine the acid and basic dissociation constants of an amino acid, and hence the isoelectric point of the acid pHmetrically.
8. Ostwald's dilution law: Dissociation constant of acetic acid conductometrically
9. Determination of solubility product and solubility of silver chloride potentiometrically using concentration cell.
10. Determination of strength of a given dibasic acid by conductometric titration.
11. Study the alkaline hydrolysis of ethyl acetate conductometrically.
12. To determine the amount of Fe (III) present in the given solution by using salicylic acid by colorimetric titration (Static method) at $\lambda = 525$ nm.
13. Determination of order of reaction for ion exchange reaction.
14. Extraction efficiency of solute from a solution by immiscible solvent method
15. Determination of the formation constant of silver-ammonia complex and stoichiometry of the complex potentiometerically.
16. Determination of flash point, fire point of a lubricant.

TEXTBOOKS

1. *Alexander Findlay, 'Practical physical chemistry', 9th edition, Wiley, 1972.*
2. *R.C. Das and B. Behera, 'Experimental Physical Chemistry', Tata McGraw-Hill, 1983.*

REFERENCES

1. *J.B. Yadav, 'Advanced Practical Physical Chemistry', Krishna Prakashan Media, 29th edition, 2010.*
2. *Francis William Gray, 'A Manual of Practical Physical Chemistry' Macmillan and Co., Limited, 1914.*

22CHY584 Inorganic Quantitative Analysis Lab 0 0 5 2

1. Estimation of Calcium (Permanganometry)
2. Estimation of Barium (Iodometry)
3. Estimation of Calcium as Calcium Carbonate (Gravimetry)
4. Estimation of Zinc using oxine (Gravimetry)
5. Estimation of Iron as Ferric Oxide (Gravimetry)
6. Analysis of Brass
7. Estimation of Copper and Nickel in a Mixture
8. Estimation of Copper and Iron in a Mixture
9. Preparation and Determination of Ferrous Oxalate
10. Estimation of Different Types of Hardness in the Given Water Sample
11. Estimation of Different Types of Alkalinities in the Given Water Sample
12. Estimation of Dissolved Oxygen in the Given Water Sample
13. Complexometric Estimations
14. Analysis of some typical alloys such as brass, bronze and type metal.
15. Ion exchange methods of analysis: (i). Determination of capacity of an ion exchange resin. (ii). Separation of Zinc and Magnesium on an anion exchange resin and estimation of Mg^{2+} and Zn^{2+}.

TEXTBOOKS

1. *G. Svehla, 'Vogel's Qualitative Inorganic Analysis', 7th Edition', Prentice Hall, 1996.*
2. *D.A. Skoog and D.M. West, 'Analytical Chemistry - An Introduction', 4th Edition, CBS Publishing Japan Ltd., 1986.*

REFERENCES

1. *E.J. Meehan, S. Bruckenstein and I.M. Kolthoff and E.B. Sandell, 'Quantitative Chemical Analysis', 4th Edition, The Macmillan Company, 1969.*
2. *R.A. Day (Jr) and A.L. Underwood, 'Quantitative Analysis', 6th Edition, Prentice Hall of India, 1991.*

22CHY605 Advanced Physical Chemistry IV 3 1 0 4

Evaluation Pattern:

Assessment	Internal	External
Periodical 1 (P1)	15	
Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	
End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1 Surface Chemistry

Different types of interfaces, molecular and atomic surface structure, surface chemical reactions, surface tension of solutions, surface excess, thermodynamics of surfaces, Gibbs equation and its derivation, surface films, surface potential.

Adsorption by solids, Langmuir isotherm - its kinetic and statistical derivation, Freundlich equation, multilayer adsorption, BET isotherm - its kinetic derivation, measurement of surface area.

Colloids - their preparation, purification, stability & electro kinetic phenomena, Donnan membrane equilibrium, micro and nano emulsions.

Surface analysis using photoelectron spectroscopy, surface imaging techniques like SEM, TEM, AFM etc., sputter coating, ion beam principles, design of surfaces with novel properties.

Unit 2 Electrochemistry I

Review of Faraday's laws, conductivity of electrolytes, ionic mobility, transference number, Kohlrausch law, pH of acids, bases and buffers, solubility product and salt hydrolysis and Ostwald's dilution law. Deviations from the Ostwald's law, activity and activity coefficients in electrolytic solution, modern theory of conductance of strong electrolytes and its tests and improvements, Debye-Huckel-Onsager equation –

theory of mean activity coefficients of strong electrolyte – Debye-Huckel limiting law and its testing and improvement.

Unit 3 Electrochemistry II

Electrochemical cells, standard electrode potentials, reversible cell, concentration cells with and without Electrochemical cells, standard electrode potentials, reversible cell, cell notation and calculation of emf – variation of potential with concentration, pressure and temperature – concentration cells with and without transference, liquid junction potential – its calculation and elimination - thermodynamics of cell reactions and equilibrium constant - applications of e.m.f. measurements, potentiometric measurement of pH – reference electrodes - glass and quinhydrone electrodes and their performance and limitations, ion selective electrodes – biomembranes, interfacial region – electrical double layers and their structure – Helmholtz-Perrin, Gouy-Chapman and Stern models - charge transfer across interfaces, mass transport – diffusion and convection controlled transport – irreversible electrode processes - activation, concentration and IR polarisation, decomposition potential, Butler-Volmer equation - overpotential (hydrogen, oxygen and metal decomposition overvoltage), theories of overvoltage, Tafel equation, and Tafel plots – corrosion andits rate from Tafel equation.

Unit 4 Chemical Kinetics I

Reaction rates and order of reactions, determination of order of reactions, complex reactions, reversible, consecutive and concurrent reactions, reactions of variable order, steady state treatment, reaction mechanism and molecularity, theories of unimolecular reactions and termolecular reactions, Arrhenius equation, collision theory and transition state theory, comparative study of the theories of reaction rates, free energy of activation, effect of solvent on rate of reactions, ionic reactions and effect of ionic strength - salt effect, effect of pressure on velocity of gas reactions.

Unit 5 Chemical Kinetics II

Reaction dynamics, fast reactions, flash photolysis and relaxation methods, catalysis and inhibition, homogeneous catalysis, acid, base and enzyme catalysis, kinetics of enzyme - catalysed reaction - the Michaelis-Menten equation. Photochemical kinetics, steady state treatment of photochemical reactions, Semenov-Hinshelwood theory of chain reactions and explosions, free radical reactions - the Rice-Herzfeld mechanism.

TEXTBOOKS

1. *Gilbert W. Castellan, "Physical Chemistry", 3rd Edition, Narosa Publishing House, 2004.*
2. *K. J. Laidler, 'Chemical-Kinetics', 3rd Edition, McGraw Hill, New York, 2004.*
3. *An introduction to Electrochemistry, Samuel Glassstone (*2007)

REFERENCES

1. *W. J. Moore and R. G. Pearson, 'Kinetics and Mechanism', 2nd edition, Wiley, 1981.*
2. *Physical Chemistry, Peter Atkins, Julio D Paula, OUP Oxford; 9 edition (19 November (2009)*
3. *Textbook of Physical Chemistry, Samuel Glassstone*, D. Van Nostrand company, inc; 2nd edition (1946)
4. *John O'M. Bockris, Amulya K.N. Reddy, Modern Electrochemistry 1: Ionics, 2nd Edition, Springer, 1998*
5. *John O'M. Bockris, Amulya K.N. Reddy, Maria E. Gamboa-Aldeco, Modern Electrochemistry 2A: Fundamentals of Electrodics, 2nd Edition, Springer, 2001*

22CHY606 Advanced Organic Chemistry IV 3 1 0 4

Evaluation Pattern:

Assessment	Internal	External
Periodical 1 (P1)	15	
Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	
End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1 Retrosynthesis and Synthetic Strategies

Basic principles and terminologies of retrosynthesis: design and selection of appropriate organic reactions, retrosynthetic analysis - functional group interconversions, protection of functional groups, synthetic equivalent groups, convergent synthesis, disconnection approach: one group and two group C-X disconnections, one group C-C and two group C-C disconnections. Amine and alkene synthesis: important strategies of retrosynthesis, enantioselective synthesis of Corey lactone, longifolene and luciferin. Umpolung equivalent- Peterson olefination, enolate formation, Ireland method. Synthetic strategies: functional group inter-conversion – conversion of one functional group to other. Nitrogen, oxygen, sulphur protection and deprotection of hydroxyl, carboxyl, carbonyl, and amino groups, chemo and region selective protection and deprotection, utilization of protection groups in organic synthesis.

Unit 2 Oxidation and Reduction

Survey of organic reactions with special reference to oxidation and reduction. Metal based and non-metal based oxidations of (a) alcohols to carbonyls [(Chromium-John's oxidation, Collin's oxidation, Sarrett oxidation), manganese, aluminium and DMSO (Swern oxidation, Moffatt – Pfitzner oxidation, Kornblum oxidation, Corey-Kim oxidation)] alkenes to diols (manganese and osmium based) - Prevost reaction and Woodward modification, alkenes to carbonyls with bond cleavage (manganese based, ozonolysis), alkenes to alcohols/carbonyls without bond cleavage hydroboration-oxidation, Wacker oxidation, selenium based allylic oxidation. ketones to ester/lactones- Baeyer-Villiger oxidation. Catalytic hydrogenation (heterogeneous: palladium/platinum /rhodium/nickel. Homogeneous: Wilkinson). Metal based reductions - Birch reduction, pinacol formation, acyloin formation, enzymatic reduction using Baker's yeast.

Unit 3 Organometallic Reagents

Preparation, properties and reactions of organolithium, organoboron, organosilicon, organotin, organozinc and organomagnesium, organocadmium, organomercury reagents. Preparation and reactions of organocopper, organopalladium - Wacker process – coupling and cross coupling, carbonylation reaction. Organonickel, organocobalt, organorhodium and organoruthenium reagents and their applications. Olefin metathesis reaction.

Unit 4 Synthetic Reagents

Hydride transfer reagents from Group III and Group IV in reductions - $LiAlH_4$, DIBAL-H, Red-Al, $NaBH_4$ and $NaCNBH_3$, selectrides, trialkyl silanes and trialkyl stannane. Aluminium isopropoxide (oxidation and reduction). Ylides: reactions involving phosphorus and sulphur. Reagents such as NBS, DDQ and DCC. Gilmann reagent. DMAP-Borane, $DMF/POCl_3$ PCC, DEAD, TEMPO, DMSO, $Cu(OAc)_2$, $NaIO_4$, B_2H_6/H_2O_2, Reduction with N_2H_4 and N_2H_2.

Unit 5 Ring Closure Reactions

Macrolactonisation, iodolactonisation, selenolactonisation, cycloadditions induced by sulphur reagents, α-halogenations, sulphenylation and selenylation of carbonyl compounds, reactions by metallocarbenes - Grubbs and Schrock catalyst.

TEXT BOOKS

1. *Modern Organic Synthesis, Dale L. Boger, The Scripps Research Institute, Rush Press, San Diego, California, 2001*
2. *Francis A. Carey and Richard J. Sundberg, "Advanced Organic Chemistry - Part B: Reactions and Synthesis", 5th Edition, Springer, 2008.*
3. *R.O.C. Norman and J.M. Coxon, "Principles of organic synthesis", CRC press, 2014*

REFERENCES

1. *Stuart Waren, Designing Organic Synthesis: A programmed introduction to the synthon approach, JOHN WILEY & SONS, 2nd edition, 2008*
2. *Name Reactions: A collection of detailed Mechanisms and synthetic applications, Jie Jack Li, Springer, fourth edition (expanded edition), 2009.*
3. *Michael B Smith, "March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure", 7th edition, Wiley (2015).*
4. *Francis A. Carey and Richard J. Sundberg, "Advanced Organic Chemistry - Part A: Structure and Mechanisms", 5th Edition, Springer, 2008*

22CHY603 Advanced Inorganic Chemistry III 3 0 0 3

Solid State Chemistry and Material Science

Evaluation Pattern:

Assessment	Internal	External
Periodical 1 (P1)	15	
Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	
End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1 Introduction to Crystal Systems

Introduction to solids - solid state chemistry, close packing, hcp, fcc, density, coordination numbers, tetrahedral and octahedral holes, body centred and primitive structures, symmetry, proper rotation, mirror planes, inversion, improper axis symmetry elements, symmetry in crystals, Schoenflies and Hermann-Mauguin notations, unit cells, glide plane, screw axis, atom occupancy in cubic unit cells, seven crystal systems/classes, space groups, Miller indices, Bravais lattices, reciprocal lattice, inter-planar spacing in different crystal systems, fractional coordinates, ionic solids, structures of CsCl, NaCl, NiAs, zinc blende and wurtzite structures, MX_2 type solids, fluorite and antifluorite structures, $CdCl_2$ and CdI_2 structures, rutile and anti-rutile, ReO_3, spinel and inverse spinel, perovskite structures, ionic radii, crystal radii, radius ratio, extended covalent array, diamond, graphite. *Liquid crystals*: Mesomorphic state, types, examples and applications of liquid crystals.

Unit 2 Bonding in Solids and Electronic Properties

Bonding in crystals, metallic bonding, ionic bonding, covalent bonding, silicates, Born-Haber cycle, Hess's law, lattice energy (L) and calculation of L, free electron theory, density of states, electronic conductivity, molecular orbital theory, overlap and bonding, linear chain of H atoms, LCAO, Fermi Level, conductors, insulators and semiconductors, n- and p-type semiconductors, bands in compounds, band-gap energy, direct and indirect band gaps in semiconductors, band-gap measurements, electrical conductivity, photo-conductivity.

Unit 3 Magnetic and Optical Properties of Solids

Behaviour of substances in magnetic field, magnetic moments, paramagnetism, diamagnetism, ferro- and anti-ferromagnetism, ferrimagnetism, effects of temperature of magnetism, Curie & Curie-Weiss laws; mechanism of ferro- and anti-ferromagnetic ordering, super exchange. Luminescence and phosphorescence of solid materials, phosphors, lasers, non-stoichiometry and its effect in properties of solids, electronic properties of non-stoichiometric oxides. Defects in solids, Schottky defects, Frenkel defects, doping in crystals and colour features, ruby, diamond, organic conductors, preparation, mechanism of conduction in organic semiconductors, photoconductivity of polymers.

Unit 4 Materials Science - Structure and Properties

Solid materials of importance. Structure and properties of SiO_2, ZrO_2, SiC, BN, ZnO, TiO_2, CdS, CdTe, GaAs, MoS_2. Band-gap properties of semiconductors like ZnO, TiO_2, CdS, CdSe, CdTe, GaAs, MoS_2 and $(CH_3NH_3)[PbX_3]$ - type perovskites. Photo-catalytic properties of ZnO and TiO_2 – principle and applications. Inorganic-organic hybrid materials. High Tc superconductors (HTS) like Bi-Sr-Ca-Cu oxide based HTS (BSCCO) and Y-Ba-Cu-oxide (YBCO), their structure and properties. Metal-organic framework (MOF) materials, special features of MOF materials. Synthesis, special features and properties of MOF materials like HKUST-1 and MOF-8. Gas storage and emission properties of MOF materials. MOFs as sensors, MOFs in pharmaceuticals. Zeolites, their special features and properties.

Unit 5 Materials Science-Synthesis, Processing and Characterization

Sol and gel, their properties, xerogels. Sol-gel synthesis - synthesis of SiO_2 and TiO_2 through sol-gel process. Calcination and sintering. Characterization of processed materials, PXRD, IR, Raman, UV-visible and solid-state NMR spectral techniques. Understanding morphological features through, SEM, EDAX and TEM methods. Chemical vapour deposition (CVD) method. Solid state synthesis, synthesis of High Tc superconducting materials like YBCO and BSCCO. Synthesis of inorganic-organic hybrid materials. Solvo-thermal and high-pressure synthesis.

TEXTBOOKS:

1. *L V Azaroff, 'Introduction to Solids' , Tata McGraw-Hill publishing company*
2. *L. E. Smart and E. A. Moore, Solid State Chemistry – An Introduction, 4th Edition, CRC Press, 2016.*

3. *A. R. West, Solid State Chemistry and its Applications, Wiley, 2014*
4. *C N R Rao, K Biswas, Essentials of Inorganic Materials Synthesis, John Wiley, 2014*
5. *C N R Rao Chemical Approaches to Synthesis of Materials, Wiley, 1994*

REFERENCES

1. *D. Jiles, "Magnetism and Magnetic Materials", Chapman and Hall, London, 1991.*
2. *R. E. Hummel, "Electronic Properties of Materials", 3rd ed., Springer-Verlag, New York, 2001.*
3. *Schubert, U. and Hüsing, N, Synthesis of Inorganic Materials, 3rd edition, VCH-Wiley Verlag GmbH, Weinheim, 2012*
4. *W.D. Kingery, H.K. Dowen and R.D. Uhlman, Introduction to Ceramics, John Wiley.*
5. *F.H. Norton, Elements of Ceramics.*
6. *M.W. Barsoum, Fundamentals of Ceramics, McGraw Hill.*
7. *Material Science and Engineering, S.K. Hajra Choudhury, Indian Book Dist.*
8. *B D Fahlman, Materials Chemistry, 2nd Edition, Springer, 2011*
9. *Stefan Kaskel, The Chemistry of Metal–Organic Frameworks: Synthesis, Characterization, and Applications, Wiley-VCH Verlag GmbH, 2016*

22CHY604 Advanced Inorganic Chemistry IV 3 0 0 3

Bio-Inorganic Chemistry

Evaluation Pattern:

Assessment	Internal	External
Periodical 1 (P1)	15	
Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	
End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1 Basics in Bio-Inorganic Chemistry

Essential elements in biological systems, transport of ions across biological membranes, active and passive transport, metal transport and metallochaperons, Na^+/K^+ pump and active transport. Metal complexation with biological molecules. Electron transport in biology, electron transport chain (ETC), role of ETC in biological systems. Amino acids, peptides and proteins, primary and secondary structure of proteins, α-helix and β-sheets forms of proteins and their special features; tertiary and quaternary structures of proteins the type of molecular interactions involved in them. Reactive oxygen species (ROS), generation and function of organic free radicals, action of ROS in biological systems, oxidative stress, antioxidants. Photosynthesis, PS-I and PS–II.

Unit 2 Oxygen Take-up, Transport and Storage Proteins

Porphine, corrin, corrole, chlorin and bacteriochlorin. Myoglobin (Mb) and haemoglobin (Hb), their prosthetic groups and functions, mechanism for reversible binding of O_2 in Mb and Hb. Cooperative effect in Hb and its consequence. Behaviour of bound O_2 to Fe(II). Difference between O_2 and CO binding to Hb and Mb, CN^- poisoning. Structure and functions of haemerythrin (Hr) and haemocyanin (Hc), O_2 binding nature in Hr and Hc, electron transfer processes in them. Cytochromes and their role in biology, cytochrome P-450, cytochrome C-oxidase and oxygen transfer from O_2 to non-activated substrates, monooxygenases, methane monooxygenase (MMO). Fe-S and other non-haeme iron proteins, ferredoxins - their structure and special properties, transferrin, ferritin, siderophores, enterobactin, uptake, transport and storage of iron. Sickle-cell anaemia

Unit 3 Metalloenzymes

Catalases – structure and properties reaction mechanism. Peroxidases- glutathione peroxidase, HRP, structure and properties and enzyme reaction mechanism. Cytochrome c peroxidase and lignin peroxidase. Copper enzymes-structure and function, azurin, plastocyanin. Type I, II and III copper proteins. Superoxide dismutase (SOD) - structure and enzymatic reaction mechanisms. Tyrosinase, reaction mechanism. Zn-containing enzymes, carbonic anhydrase and carboxy-peptidases-structure and enzymatic reactions. N_2

fixation, nitrogenase enzyme, Fe-S clusters, Fe-protein structure, Mo-Fe protein structure, P-cluster and M-centre, their model compounds.

Unit 4 Other Metalloproteins and Biomimetic Compounds

Zn in biological systems, Zn-finger proteins – structural features and properties, classifications and their roles in biological systems. Ca^{2+} binding proteins, calmodulins. Porphyrins (H_2P) and metalloporphyrins (MP), spectral, fluorescence and redox properties of H_2P and MP. Biomimetic compounds. Fe(II), Co(II) and Cu(II) based model compounds model compounds of Mb and Hc – 'picket-fence' porphyrin and its special features. Natural and synthetic ionophores, crown ethers, interaction and uptake of alkali metal and alkaline earth metal ions with crown ethers, cryptands and cryptates, calixarenes and their special properties, cyclo-dextrins and their special properties.

Unit 5 Metals in Medicine and Other Roles

Metal ion based (Pt, V, Au) drugs, anticancer agents. Cis-platin and its properties, ruthenium - based anticancer agents, chelation therapy, macrocyclic antibiotics. Role of Mn, Ni, Mo and Cr in biological systems, metal toxicity and homeostasis, therapeutic complexes. Diseases caused by both excess and deficiency of metal ions, thalassaemia, Wilson disease. DNA intercalators, diagnostic agents, MRI imaging and contrast agents, the role of Gd^{3+} and other metal ions as contrast agents. Photodynamic therapy (PDT), principles and applications.

TEXTBOOKS

1. *J.E. Huheey, R.A. Keiter, R.L. Keiter, Inorganic Chemistry-Principles of Structure and Reactivity, 4th Edn., Prentice Hall, 1997.*
2. *F.A. Cotton, G. Wilkinson, C.A. Murillo, M. Bochmann, Advanced Inorganic Chemistry, 6th Edn., Wiley-Interscience, 1999.*
3. *P. Atkins, T. Overton, J. Rourke, M. Weller, F. Armstrong, Shriver and Atkins Inorganic Chemistry, 4th Edn., Oxford University Press, 2006.*

REFERENCES

1. *S. J. Lippard, J. M. Berg, Principles of Bioinorganic Chemistry, University Science Books, 1994.*
2. *J. D. Atwood, Inorganic and Organometallic Reaction Mechanism, 2nd Edition., Wiley-VCH, 1997.*
3. *B.E. Douglas, D.H. McDaniel, J. J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn., Wiley-India, 2007.*
4. *W. Kaim, B. Schwederski, Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, John Wiley & Sons, 1994.*
5. *M. N. Hughes, The Inorganic Chemistry in Biological Processes, Wiley (1981)*

22CHY681 Organic Qualitative Analysis Lab 0 0 5 2

Separation of binary mixtures

Includes separation, preliminary investigations, determinations of saturation/unsaturation, detection of elements by Lassaigne's test, functional group identification, derivative preparation, determination of melting points of the derivatives and calculation of Rf values from TLC

1. The following mixtures can be given:

a. Acid and hydrocarbon
b. Phenol and aldehyde
c. Phenol and acid
d. Phenol and amine
e. Acid and ester
f. Halo compound and aldehyde
g. Acid and aldehyde
h. Amine and aldehyde
i. Amine and ketone

j. Alcohol and hydrocarbon

2. Thin layer chromatography to determine Rf values of compounds:

a. 2-nitroaniline
b. 4-nitroaniline
c. Cinnamic acid and 2-nitroaniline
d. Acetophenone
e. Ethyl benzoate

3. Simple column chromatography to separate the components of binary mixtures:

(a) Hydrocarbon and ester
(b) Aldehyde and amine

REFERENCES

1. *P.W.G. Smith, A.J. Hannaford, B.S. Furnis and A.R. Tatchell, "Vogel's Textbook of Practical Organic Chemistry", ELBS/Longman, 1989.*
2. *Ralph L. Shriner, Christine K.F. Hermann, Terence C. Morrill, David Y. Curtin, Reynold C. Fuson, 'Systematic Identification of Organic Compounds', John Wiley & Sons, 2003.*
3. *Mann and Saunders, 'Practical Organic Chemistry', Pearson edition, 2009*

22CHY682 Instrumental and Analytic Methods lab 0 0 5 2

1. Determination of strengths of halides in a mixture potentiometrically**.**
2. To find the redox potential of the given sample using cyclic voltametry.
3. Determination of half wave potential of Cd & Zn by polarography.
4. Determination of pKa of an indicator in aqueous and micellar medium using UV-Vis spectroscopy.
5. Determination of stoichiometry and stability constant of inorganic (ferric-salicylic acid) and organic (amineiodine) complexes using UV–Vis spectroscopy.
6. Determination of copper and cadmium in a mixture by electrogravimetry.
7. Determination of rate constant for enzyme kinetics-inversion of sucrose.
8. Determination of a molecular weight of a solute using Beckmann thermometer.
9. Refractometric determination of composition of solutions.
10. Spectrophotometric determination of the amount of Cr (VI) in the given solution as dichromate by the method of least squares.
11. Spectrophotometric determination of the amount of fluoride present in the given solution.
12. Determination of the amount of acetic acid in a sample of vinegar by potentiometric titration with a standard base using quinhydrone.
13. Determination of vitamin C content of a given tablet pHmetrically.
14. Spectrophotometric determination of Fe in Water Sample using Standard Addition

TEXTBOOKS

1. *Alexander Findlay, 'Practical Physical Chemistry', 9th edition, Wiley, 1972.*
2. *R.C. Das and B. Behera, 'Experimental Physical Chemistry', Tata McGraw-Hill, 1983.*

REFERENCES

1. *J.B. Yadav, 'Advanced Practical Physical Chemistry', Krishna Prakashan Media, 29th edition, 2010.*
2. *Francis William Gray, 'A Manual of Practical Physical Chemistry' Macmillan and Co., Limited, 1914*

22CHY631 Applied Electrochemistry 3 0 0 3

Evaluation Pattern:

Assessment	**Internal**	**External**
Periodical 1 (P1)	15	
Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	
End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1 Electrodics: Electron transfer under an interfacial electric field, A two-way traffic across the interference: equilibrium and exchange current density. Dependence of the electrochemical reaction rate on overpotential - quantitative version of the Butler Volmer equation. Electrode kinetics involving the semiconductor/solution interface. Techniques of electrode kinetics - preparation of electrode surface. Microelectrodes - applications

Unit 2 Industrial Cathodic Process - Electrodeposition of copper, nickel and chromium over mild steel – zinc plating on MS – decorative plating of silver and cold – nano plating and microstructure of deposits - Tests for adhesion, hardness, thickness, uniformity and corrosion resistance of the electro deposits - post plating passivation processes - barrel plating of small components - Electroless deposition of nickel, copper, gold on metal components – making of waveguides and plated through hole boards -

Unit 3 Industrial Anodic Processes: Anodizing of aluminium and its alloys – baths used, operating conditions and sequence determination of thickness – industrial applications - nano anodizing of titanium, and tantalum – application to sensor field - Electropolishing of ferrous and non-ferrous metals and alloys - mechanism of electropolishing –Electrochemical etching of ferrous and non-ferrous metals – Special processes: Electrolysis of water – electrowinning of aluminium and sodium – electrolysis of brine-photoelectrochemistry

Unit4 Electrochemical Energy Systems: Primary batteries: Zinc-carbon (Leclanche type), zinc alkaline (Duracell),; lithium primary cells - liquid cathode, solid cathode and lithium-ferrous sulphide cells Secondary batteries: Lead acid and VRLA (valve regulated [sealed] lead acid), nickel-cadmium, nickel-zinc, nickel-metal hydride batteries, lithium ion batteries, ultra-thin lithium polymer cells (comparative account) Advanced Batteries for electric vehicles, requirements of the battery - sodium-beta and redox batteries. Reserve batteries, thermally activated batteries - remote activation - pyrotechnic materials: Fuel Cells: principle, proton-exchange membrane (PEM), direct methanol (DMFC), molten carbonate electrolyte (MCFC) fuel cells and outline of biochemical fuel cells.

Unit5 Electrochemical Sensors: Potentiometric sensors, solid state potentiometric chemical sensors, polymeric membrane sensors, ion selective field effect transistor, application, hydrovolumetric technique-hydrodynamic voltammetric-application, voltammetric sensors-electrode modification application, optical sensors - bioamperometric titration. Methods involving forced convection - hydrodynamic methods

TEXT BOOKS

1. *Allen J. Bard and Larry R. Faulkner, 'Text book for Electrochemical Methods', 2nd edition, Wiley, 2000.*
2. *Derek Pletcher and Frank C. Walsh, 'Industrial Electrochemistry', Blackie Academic and Professional, (1993).*

REFERENCES

1. *Christopher M A, Brett, 'Electrochemistry – Principles, Methods and Applications', Oxford University, (2004).*
2. *Watanabe T, 'Nano-plating: microstructure control theory of plated film and data base of plated film microstructure', Elsevier, Oxford, UK (2004).*
3. *Kanani N, 'Electroplating and electroless plating of copper and its alloy', ASM International, Metals Park, OH and Metal Finishing Publications, Stevenage, UK (2003).*
4. *Curtis, 'Electroforming', London, (2004).*
5. *Rumyantsev E and Davydov A, 'Electrochemical machining of metals', Mir, Moscow, (1989).*
6. *Peter G Sheasby 'Basics of Aluminium Anodizing', Banbury, Oxon (2001)*
7. *Robert Brugger 'Nickel Plating' Robert Draper Ltd, Teddington, (1970)*
8. *J. K. Dennis, T. E. Such, 'Nickel and Chromium Plating, Third Edition' Woodhead Publishing Series in Metals and Surface Engineering, 3rd Edition, (1993)*

22CHY632 Bioanalytical Chemistry 3 0 0 3

Evaluation Pattern:

Assessment	Internal	External
Periodical 1 (P1)	15	

Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	
End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1 Enzymes

Enzyme nomenclature, enzyme commission numbers, enzymes in bioanalytical chemistry, enzyme kinetics - enzyme activators, enzyme inhibitors.

Unit 2 Quantification of Enzymes and Their Substrates

Instrumental methods, optical detection - absorbance, fluorescence, luminescence, nephelometry electrochemical detection - amperometry, potentiometry, conductometry, other detection methods - radiochemical, manometry, calorimetry.

Unit 3 Immobilized Enzymes

Immobilization methods - nanopolymerizing covalent immobilization, Crosslinking with bifunctional reagents. Properties of immobilized enzymes, immobilized enzyme reactions, theoretical treatment of packed bed enzyme reactors.

Unit 4 Antibodies

Structural and functional properties of antibodies, Polyclonal and monoclonal antibodies Antibody-antigen interactions, analytical application of secondary antibody-antigen.

Unit 5 Biosensors

Response of enzyme-based biosensors, examples of biosensor configuration, ferrocene-mediated amperometric glucose sensor, potentiometric biosensor for phenyl acetate, potentiometric immunosensor for digoxin, optical biosensor for glucose based on fluorescence energy transfer, piezoelectric sensor for nucleic acid detection, enzyme thermistors.

TEXTBOOKS

1. *Susan R. Mikkelsen, and Eduardo Corto´n 'Bioanalytical Chemistry', 1st edition, Wiley Interscience, 2003.*
2. *Andres Manz, Nicole Pamme and Dimitri Lossifidis, 'Bioanalytical Chemistry', World Scientific Publishing Company, 2004.*

REFERENCE

1. *Robert W. Cattrall, 'Chemical Sensors', Oxford University Press, 1997.*

22CHY633 Chemistry of Biomolecules 3 0 0 3

Evaluation Pattern:

Assessment	**Internal**	**External**
Periodical 1 (P1)	15	
Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	
End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1 Amino acids, Proteins and Peptides

Classification, Stereochemical aspects, physical properties, Ionic properties, spectral properties, essential and non-essential amino acids, chemical reactions of amino acids, Industrial preparation and chemical synthesis of amino acids. Ionic properties of proteins, protein structure, protein purification, protein structure determination, proteomics and protein function, solid phase peptide synthesis, biologically

important peptides.

Unit 2 Enzymes

Introduction to Enzymes, Classification of enzymes, mechanism of enzyme action, immobilized enzymes and enzyme technology, enzyme- analogue built polymers, design of molecular clefts, enzymes in synthetic organic chemistry. Enzymes in biological systems

Unit 3 Molecular Biology and Bioinformatics

Structure of nucleic acids, genes and genome complexity, functions of nucleic acids, isolation and separation of nucleic acids, molecular analysis of nucleic acid sequences, nucleotide sequencing of DNA.

Unit 4 Immunochemical Techniques

Production of antibodies, purification and fragmentation of immunoglobulins, immunoprecipitation, labelling antibodies, immunoblotting, immunoassays, immunohistochemistry/cytochemistry.

Unit 5 Recombinant DNA and Genetic Analysis

Constructing gene libraries, cloning vectors, hybridization and gene probes, application of gene cloning, expression of foreign genes, pharmacogenomics.

REFERENCES

1. *Hermann Dugas, 'Bioorganic Chemistry - A Chemical Approach to Enzyme Action', 3rd edition, Springer.*
2. *Keith Wilson and John Walker, 'Principles and Techniques of Biochemistry and Molecular Biology', 6th edition, Cambridge University Press.*

22CHY634 Industrial Chemistry 3 0 0 3

Evaluation Pattern:

Assessment	Internal	External
Periodical 1 (P1)	15	
Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	
End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1 Water Treatment

Softening of water, ion exchange process, lime soda process, modified lime soda process, zeolite process, chemical and physical method of sterilization, desalination, boiler problems. Corrosion of boiler units, industrial water treatment, water analysis.

Unit 2 Fuels

Calorific value, determination of calorific value, classification of fuels, solid fuels, properties of fuels, classification of coal, coking and non-coking coals, advantages and disadvantages of solid fuels. Liquid fuels, gaseous fuels, analysis of fuel gases, distillation of petroleum. processing & purification of petroleum and petroleum products, flash point, fire point, knocking, antiknocking, cetane number, octane number, natural gasoline, cracking, polymerization, alkylation, isomerisation, rocket fuels, fossil fuels, nuclear fuels.

Unit 3 Energy Resources

Renewable and non-renewable sources of energy, conventional and non-conventional sources of energy, solar energy, solar technology, solar photovoltaic cell - application, PV lantern system, radiotelephone

system, application of solar energy, environmental implication, nuclear energy, nuclear fuel cycle in India, Energy conservation and waste heat boilers, Fuel cells, hydrogen cells.

Unit 4 Paints and Pigments

White pigment, blue, green, yellow, black and red pigments - manufacture, physical properties, characteristics, manufacture of paints, setting of paints, requirement for good paints, emulsion paint, latex paint, luminescent paint, fire retardant paints, heat resistant paints, varnishes, manufacture of varnishes, enamels, lacquers.

Unit 5 Explosives and Toxic Chemical Weapons

Introduction, classification. deflagrating or low explosives. Characteristics of explosives, nitrocellulose, PETN, DNB, TNB, TNT, picric acid, nitro glycerine, dynamite, cirdite, gun powder, RDX, EDNA, HMX, tetryl, pentyl, hexyl, dinol. toxic chemical weapons, screening smokes, incendiaries, pyrotechniques, explosives in India.

TEXTBOOKS

1. *B.K. Sharma, 'Industrial Chemistry', Goel publishing.*
2. *James A Kent, 'Riegel's Hand book of Industrial chemistry', 10th edition, Kluwer Academic/Plenum publishers, 2003.*

REFERENCES

1. *Alan Heaton, 'An Introduction to Industrial chemistry', 3rd edition, Blackie Academic and professional, 1996.*
2. *Chris A Clausen and Guy Mattson, 'Principles of industrial chemistry', 2nd edition Wiley, 1978.*
3. *Jonathan Steed, 'Core Concepts on supramolecular chemistry and nanochemistry', Wiley Eastern Publishers, 2006.*

22CHY635 Industrial Stoichiometry 3 0 0 3

Evaluation Pattern:

Assessment	Internal	External
Periodical 1 (P1)	15	
Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	
End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1 Introduction to process calculation - dimensions and systems of units - fundamental quantities of units, derived quantities, definition and units of force, volume, pressure, work, energy, power, heat-unit conversions in FPS, MKS and SI systems.

Unit 2 Mixtures and solutions - methods of expressing compositions of mixture and solutions, wet and dry basis concept. Ideal and real gas laws – gas constant – normal molal volume, calculations of pressure, volume and temperature using ideal gas law. Gas mixtures – use of partial pressure and pure component volume in gas calculations. Dissociating gases. Relation between mole%, volume% and pressure% of ideal gases, calculation of average molecular weight, density, mole%, weight% in gas mixture in SI/MKS systems – applications of real gas relationship in gas calculation.

Unit 3 Description and simple material balance calculation of physical processes such as drying, distillation, absorption, mixing, crystallization, evaporation.

Unit 4 Single stage material balance calculation of leaching and extraction, calculations involving recycling and by-passing operation - limiting reactant, excess reactant, conversion, yield and selectivity - simple numerical for finding yield, conversion and composition.

Unit 5 Calculation of material and energy balance based on reactions involving heat capacity and specific heat - mean heat capacity of gases - heat capacity of gas mixture and liquid mixture. Calculations of heat capacity by integral equation up to three terms - sensible and latent heats of fusion, sublimation,

vaporization. Calculations of standard heat of formation from heat of combustion data. Calculations for heat of reaction from heat of formation and heat of combustion data – fuels - calorific values proximate and ultimate analysis - air requirement and composition of flue gases.

TEXTBOOKS

1. *Bhatt, B.L. Vora, S.M., "Stoichiometry", 3rd Edition, Tata McGraw-Hill (1996).*
2. *Felder, R.M. and Rousseau, R.R. "Elementary Principles of Chemical Processes" 3rd Edn., John Wiley & Sons, New York 2000.*

REFERENCES

1. *Hougen O.A., Watson K.M. and Ragatz R.A., "Chemical Process Principles" Part I, CBS Publishers (1973).*
2. *Warren. K Lewis, Arthur H. Radash & H. Clay Lewis, "Industrial Stoichiometry", McGraw Hill Book C., NY 1995.*

22CHY636 Material Science and Nanochemistry 3 0 0 3

Evaluation Pattern:

Assessment	Internal	External
Periodical 1 (P1)	15	
Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	
End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1 Introduction to nanomaterials, introduction to material science, interdisciplinary nature, structure of nanomaterials, length scales, de-Broglie wavelength & exciton Bohr radius, foundations of quantum mechanics: wave function, Schrödinger equation, uncertainty principle, quantum wells, quantum wires, quantum dots, articles.

Unit 2 Nanomaterials: Synthesis, properties, size effect and properties of nanoparticles - particle size - particle shape - particle density, specific surface area and pore - composite structure, crystal structure - functionality of nanostructures and their characteristic evaluation - optical properties - catalytic property; synthesis - methods and strategies, top-down and bottom-up approaches, chemical vapor deposition, laser ablation, electric-arc, sol-gel processing, lithography - surface modification of inorganic nanoparticles by organic functional groups.

Unit 3 Surface science and characterization of nanomaterials. Electron Microscopy, MFM, SNOM, SEM, TEM, EDAX, X-ray diffraction and electron diffraction, atomic force microscopy, scanning tunneling microscopy, spectroscopy: UV-visible spectroscopy, photoluminescence spectroscopy, IR spectroscopy, FTIR and ATR, Raman spectroscopy, self-assembled monolayers.

Unit 4 Nanotechnology: applications and devices. Nanoscale materials, nano transfer printing, biomaterials applications, MEMS and NEMS, self-organization, nanoscale (opto) electronics, fullerenes, devices - actuators and motors for nano displacements, nanosensors, development of optical memory using semiconductor nanoparticles - nozzle-free inkjet technology - dendrimers and their application to organic electronics devices - nanomedicines, bio-imaging with quantum dots.

Unit 5 Environmental issues in nanotechnology. Nanoparticles and environment - nanoparticles in atmosphere - ground water, exhaust gases – waste water and indoor environments; safety of nanoparticles - problems caused by nanoparticles, safety assessment for the nanoparticles; removal of nanoparticles.

TEXTBOOKS

1. *T. Pradeep, 'Nano - The Essentials Understanding Nanoscience and Technology', McGraw-Hill Professional Publishing, 2008.*
2. *Charles P. Pool and Frank J. Ovens, 'Introduction to Nanotechnology', John Wiley and sons, 2006.*

REFERENCES:

1. *Ozin, Geoffrey Alan, Arsenault, 'Nanochemistry: A Chemical Approach to Nanomaterials', Royal Society of Chemistry, 2008.*
2. *C.N.R. Rao, A. Muller, A.K. Cheetham, 'The Chemistry of Nanomaterials: Synthesis, Properties and Applications', Wiley-Vch Verlag Gmbh & Co., 2004.*
3. *Alexei Nabok, 'Organic and Inorganic Nanostructures', Artech House, 2005.*
4. *C. Richard Brundle, Charles A. Evans Jr., and Shaun Wilson, 'Encyclopedia of Materials Characterization', Butterworth-Heinemann Publishers, 1992.*
5. *Masuo Hosokawa, Kiyoshi Nogi, Makio Naito and Toyokazu Yokoyama, 'Nanoparticle Technology Handbook', Elsevier Publishers, 2007.*

22CHY637 Medicinal Chemistry 3 0 0 3

Evaluation Pattern:

Assessment	Internal	External
Periodical 1 (P1)	15	
Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	
End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1 Medicinal chemistry: Introduction, drugs – classification of drugs – mechanism of drug action. Drug-receptor complex, nomenclature – agonist,

Unit 2 Physicochemical Properties of Drugs in Relation to Biological Action: solubility**,** partition coefficient, dissociation constant, hydrogen bonding, ionization, drug shape, surface activity, complexation, protein binding, molar refractivity, bioisosterism – stereo chemical aspects of drug action.
Enzymes, hormones and vitamins - representative cases, nomenclature, classification and characteristics of enzymes, mechanism of enzyme action, factors affecting enzyme action, co-factors and co-enzymes, enzymes in organic synthesis, mechanism of enzyme catalysis, enzyme inhibition. Hormones and vitamins – representative cases.

Unit 3 Essentials of Drug Design
Molecular mimetics, drug-lead modification, drug design using QSAR and computer assisted design, assessment of drug activity, receptors and drug action, mechanism of drug action, drug metabolism pathways, drug potentiation, drug antagonism and drug resistance

Unit 4 Medicinal Agents from Natural Products
History of the use of natural products as therapeutic agents, medicinal plants, active principle, isolation methods of alkaloids, terpenes, antioxidants, natural oils from plants

Unit 5 Medicinal Agents
Medicinal agents belonging to alkaloids, steroids, polypeptides, modified nucleic acid bases, sulphonamide and sulpha drugs, antibacterials - sulpha drugs, substituted sulphonamides, anticonvulsants, anticoagulants, antiamoebic agents, anthelmintic agents, anti-malarial agents, diuretics and cardio vascular agents, medicinal agents affecting CNS, analgesics, antipyretics, antiseptics and disinfectants, histamine and anti-histaminic agents. Infectious and non-infectious diseases (malaria, AIDS, Cancer) introduction, mechanism of action types of cure.

TEXTBOOKS

1. *John M beak and John H Block, 'T Wilson, O. Gisvold and R. F. Deorge - Text book of Organic, Medicinal and Pharmaceutical Chemistry', 7th edition, J.B. Lippincott Williams and Wilkons Company, 1977.*
2. *A. Burger, 'Medicinal Chemistry', 3rd edition, Wiley Interscience, 1970.*
3. *V.K. Ahluwalia and Madhu Chopra, 'Medicinal Chemistry', Ane Books Pvt. Ltd, 2008.*

REFERENCES

1. *V. Kothekar, 'Essentials of Drug Designing', 14th edition, Dhruv publications, 2005.*

2. *V.K. Ahluwalia, Lalita S. Kumar and Sanjiv Kumar, 'Chemistry of Natural Products', Ane Books India.*
3. *L.P. Graham 'An introduction to Medicinal Chemistry', 3rd edition, Oxford University Press, 2005*

22CHY638 Supramolecular Chemistry 3 0 0 3

Evaluation Pattern:

Assessment	Internal	External
Periodical 1 (P1)	15	
Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	
End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1 Introduction to Supramolecular Chemistry

From molecular to supramolecular chemistry: factors leading to strong binding, hydrogen bonding and stacking interactions, bottom-up approach, top-down approach, energy and signals semiochemistry, photo switching devices, electro switching devices, mechanical switching processes,

Unit 2 Processing of Energy and Signals by Molecular and Supramolecular System

Fundamental principles of photo induced electron and energy transfer, molecular electronics, molecular photonics, molecular chemionics, molecular electro photonics, molecular photochemionics.

Unit 3 Molecular Recognition

Molecular receptors: crown ethers, siderophores, cyclophanes, cyclodextrin and their application in specific recognition processes. Metal guided self-assembly reactions, molecular knot with double helical complexes, self-assembly of polynuclear metal complexes.

Unit 4 Electrochemistry of Supramolecular Systems

Electroluminescent systems as sensors and devices, Redox controlled molecular switches, biohybrid electrochemical devices, dendrimers as multielectron storage devices, redox-active Metal - Polypyridine dendrimers as light harvesting antennae.

Unit 5 Molecular Scale Mechanical Devices

Introduction to mechanical devices, spontaneous mechanical like motions, allosteric movements, tweezers and harpoons, a natural proton pump, twisters, tweezers, threading - dethreading movements, ring switching processes in rotaxanes and catenanes, molecular valves, molecular muscles.

TEXTBOOKS

1. *Vincezo Balzani, 'Supramolecular Chemistry', Kluwer Academic, 1992*
2. *Vincenzo Balzani, Alberto Credi and Margherita Venturi, 'Molecular Devices and Machines: A Journey into the Nanoworld', Wiley, 2006.*
3. *Paola Ceroni, Alberto Credi and Margherita Venturi, 'Electrochemistry of Functional Supramolecular Systems', Wiley, 2010.*

REFERENCES

1. *Jonathan W. Steed Atwood, Jerry L. Chich, 'Supramolecular Chemistry', 2nd edition, Wiley, 2009.*
2. *Fritz Vögtle and F. Alfter 'Supramolecular Chemistry: An Introduction', John Wiley & Sons, 1999.*
3. *Jean-Marie Lehn, 'Supramolecular Chemistry', RCS pubs., 2005*
4. *Jonathan Steed, David Turner and Carl Wallace, 'Core concepts in Supramolecular Chemistry and nanochemistry', John Wiley & Sons, 2007*
5. *Katsuhiko Ariga and Toyoki Kunitake, 'Supramolecular chemistry – Fundamentals and applications advanced textbook', Springer-Verlag, 2000*

22CHY639 Nanomaterials for Biomedical Applications 3 0 0 3

Evaluation Pattern:

Assessment	Internal	External
Periodical 1 (P1)	15	
Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	
End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1 Introduction to nanomaterials: size dependence of properties – surface to volume ratio and quantum confinement. Microscopic techniques to study nano structures - SEM, AFM – TEM and STM. Spectroscopic techniques to characterize nanostructures - Raman, XPS, Auger, EDAX.

Unit 2 Synthetic approaches: colloidal, self-assembly (self assembled monolayers-SAMs) and electrostatic self-assembly, electrochemical methods (cathodic and anodic processes), sol-gel, Langmuir-Blodgett (LB) technique, chemical vapour deposition, plasma arcing and ball milling, lithography.

Unit 3 Electrical, optical, mechanical, chemical and magnetic properties of nanomaterials. Surface Plasmon resonance – Fluorescence Resonance energy transfer (FRET).

Unit 4 Carbon clusters: synthesis, properties and biomedical applications of fullerenes, carbon nanotubes and graphenes. quantum dots, wells and wires (metallic and semiconducting) - preparation, properties and biomedical applications. Dendrimeric structures and their applications.

Unit 5 Biofunctionalization of nanomaterials - noncovalent assembly - covalent assembly - biofunctional nanomaterials - semiconductor nanoparticles – magnetic nanoparticles. Applications of biofunctional nanomaterials – optical and electrochemical sensing.

REFERENCES

1. *Alexei Nabok, "Organic and Inorganic Nanostructures", Artech House, Inc., 2005*
2. *Huangxian Ju, Xueji Zhang and Joseph Wang, "Nano Biosensing, Principles, Development and Application", Springer, 2011.*
3. *M. Reza Mozafari (Editor), "Nanomaterials and Nanosystems for Biomedical Applications", Springer 2007.*
4. *Zhong Lin Wang (Editor), "Characterization of Nanophase Materials", Wiley VCH, 2000.*

22CHY640 Industrial Metal Finishing Processes 3 0 0 3

Evaluation Pattern:

Assessment	Internal	External
Periodical 1 (P1)	15	
Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	
End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1 Background Theory: Review of reversible and irreversible processes - electrodes, indicator and reference - Nernst and Butler-Volmer equation - phenomenon of polarization - factors influencing - Tafel experiment and Tafel plot - Significance.

Unit 2 Electrodeposition: Industrial plating of copper-nickel (dull and bright) - chromium on mild steel –

operating conditions and sequence – pre-treatment processes - plant layout – electroplating of zinc on MS and post plating, chromating, yellow and blue passivation processes – decorative plating of silver and gold on non-ferrous metals – brief discussion on nano plating of metals and micro structure of the deposition.
Properties of deposits: tests for adhesion, hardness, thickness, uniformity and corrosion resistance of the electro deposits.
Electroless deposition: nickel, copper, gold on metal components – bath composition and operating conditions - immersion plating - plating on plastics – pre-treatment processes – long duration plating – electroforming, operating conditions and sequence.

Unit 3 Anodizing: industrial anodizing of aluminium and its alloys – baths used, operating conditions and sequence – plant layout – effect of temperature and current density on the thickness of anodic film – determination of thickness – industrial applications.
Nano anodizing of titanium, aluminium and tantalum – application to sensor field.
Plasma electrolytic oxidation: power supply requirements – baths used – process sequence for aluminium, magnesium and titanium – properties of the coating and industrial applications.

Unit 4 Electropolishing: Mechanism of electropolishing – electropolishing of ferrous and non-ferrous metals – industrial baths used – operating conditions and sequence - industrial applications.

Unit 5 Electrochemical etching: etching of ferrous and non-ferrous metals – special properties of matt and satin finish – DC and AC processes – operating conditions and sequence.
Special Topics: electrochemical and chemical metal colouring of ferrous and non-ferrous metals. Black nickel coating – hard chromium deposition – hard anodizing of aluminium – electrochemical machining of hard steels – electro-winning process – Barrel plating – electrodeposition of paint.

TEXTBOOK

1. *Derek Pletcher and Frank C. Walsh, 'Industrial Electrochemistry', Blackie Academic and Professional, (1993).*

REFERENCES

1. *Christopher M A, Brett, 'Electrochemistry – Principles, Methods and Applications', Oxford University, (2004).*
2. *Watanabe T, 'Nano-plating: microstructure control theory of plated film and data base of plated film microstructure', Elsevier, Oxford, UK (2004).*
3. *Kanani N, 'Electroplating and electroless plating of copper and its alloy', ASM International, Metals Park, OH and Metal Finishing Publications, Stevenage, UK (2003).*
4. *Curtis, 'Electroforming', London, (2004).*
5. *Rumyantsev E and Davydov A, 'Electrochemical machining of metals', Mir, Moscow, (1989).*
6. *Peter G Sheasby 'Basics of aluminium anodizing', Banbury, Oxon (2001)*
7. *Robert Brugger 'Nickel Plating' Robert Draper Ltd, Teddington, (1970)*
8. *J.K. Dennis, T.E. Such, 'Nickel and Chromium Plating, Third Edition' Woodhead Publishing Series in Metals and Surface Engineering, 3rd Edition, (1993)*

22CHY641 Biosensors: Fundamentals and Applications 3 0 0 3

Evaluation Pattern:

Assessment	Internal	External
Periodical 1 (P1)	15	
Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	
End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1 Introduction to biosensor – classification based on the signal transduction and biorecognition element. Enzymatic and non-enzymatic sensors, DNA and protein-based sensors - immunosensors.

Unit 2 Biosensing using nanomaterials: concepts of surface to volume ratio, quantum confinement, surface plasmon resonance, fluorescence, chemiluminescence and electroluminescence and FRET in biosensing. Application of metal, semiconducting quantum dots, carbon nanotubes, graphene and carbon dots in biosensing.

Unit 3 Electrochemical principle in biosensing: principles of potentiometry, voltammetry, amperometry and impedimentary in biosensing. Principle, fabrication and working of optical, electrochemical biosensors. Construction and working of potentiometric, amperometric and impedemetric sensors. Development and applications of piezoelectric sensors.

Unit 4 Optical and electrochemical sensors for glucose, vitamins, cholesterol, dopamine, nitric oxide, nitrates, and pesticides. Biocompatibility of sensors.

Unit 5 Biochips and wearable devices: lab-on-a-chip - fabrication of microfluidics- lithography, wearable sensors, epidermal electronic system, lab-on-skin-devices.

REFERENCES

1. *Xueji Zhang, Huangxian Ju, Joseph Wang, "Electrochemical Sensors, Biosensors and Their Biomedical Applications", Elsevier, 2008*
2. *Joseph Wang, "Analytical Electrochemistry", Wiley, 2006*
3. *Huangxian Ju, Xueji Zhang, Joseph Wang, "Nano Biosensing: Principles, Development and Application", Springer, 2011.*
4. *Peter Grundler, "Chemical Sensors – An Introduction for Scientists and Engineers", Springer-Verlag, Berlin Heidelberg, 2007*
5. *Arben Merkoci, "Biosensing using nanomaterials" Wiley, 2009.*

22CHY642 Computational Chemistry 3 0 0 3

Evaluation Pattern:

Assessment	Internal	External
Periodical 1 (P1)	15	
Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	
End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1 Introduction

Introduction to computational chemistry (molecular modelling), questions commonly investigated computationally, principle and application of methods (tools) of computational chemistry - molecular mechanics, ab initio method, semiempirical methods, density functional theory and molecular dynamics, STOs, GTOs, basis sets, specification of molecular geometry using Cartesian coordinates and internal coordinates, Z-matrix, Z-matrix of simple molecules (water, ethanol), potential energy surface (PES), potential energy surface of diatomic molecules and triatomic molecules (H_2O and HOF) - hypersurface and process of "slicing", stationary points on a potential energy surface - potential energy surface of the isomerization reaction of ozone to isoozone, stationary points (ozone, isoozone and transition state), intrinsic reaction coordinate, minimum, relative minimum, saddle-shaped surface, saddle point, higher-order saddle point and mathematical treatment of stationary points, Born-Oppenheimer approximation and its significance and frozen-nuclei energy.

Unit 2 Molecular Mechanics

Introduction to molecular mechanics, forcefield, developing a force field - expression for potential energy of a molecule, bond stretching term, angle bending term, torsional term and nonbonded interaction term, parameterizing a forcefield – parameterizing bond stretching term, angle bending term, torsional term and

nonbonded interaction term, calculation using forcefield - compare the energies of two 2, 2, 3, 3-tetramethylbutane geometries, illustration of application (use) of molecular mechanics - calculation of geometries and energies of small-sized and medium-sized molecules, polymers and transition states (transition state for the Diels-Alder reaction of butadiene with ethene to form cyclohexene), in organic synthesis for predicting the more suitable path for carrying out the synthesis and calculation of normal-mode vibrational frequencies for characterizing a species as a minimum or a transition state or higher-order saddle point, for obtaining zero-point energies to correct frozen-nuclei energies and for interpreting or predicting IR spectra, strength (merit) and weakness (demerit) of molecular mechanics.

Unit 3 Semiempirical Methods - Part 1

Introduction to semiempirical (SE) methods, Simple Huckel Method (SHM) - theory - expression for calculating energy of a molecular species, expression for molecular wave function based on LCAO approximation, secular equations and the single matrix equation, H, C, S and ε matrices and their interpretation, the values of H_{ij} as zero, coulomb integral α and bond integral β and their physical significance, the H matrix in terms of α, β and zero for ethene system(ethene neutral molecule, ethene radical cation and ethene radical anion), propenyl system (propenyl cation, propenyl neutral radical and propenyl anion) and cyclobutadiene system (square cyclobutadiene dication, square cyclobutadiene neutral molecule and square cyclobutadiene dianion), the H matrix in terms of zero, $\alpha = 0$ and $\beta = -1$for ethene systems (ethene neutral molecule, ethene radical cation and ethene radical anion), propenyl system (propenyl cation, propenyl neutral radical and propenyl anion) and cyclobutadiene system (square cyclobutadiene dication, square cyclobutadiene neutral molecule and square cyclobutadiene dianion), result of diagonalization of the H matrices written for ethene system, propenyl system and cyclobutadiene system, molecular orbital energy level diagrams and expressions for energy and molecular wave functions for ethene system, propenyl system and cyclobutadiene system based on the result of diagonalization of the H matrices, and molecular orbital energy level diagrams for ethene system, propenyl system and cyclobutadiene system showing ground state and excited state electronic configurations.

Unit 4 Semiempirical Methods - Part 2

Application of SHM - nodal properties of molecular orbitals and Woodward-Hoffmann orbital symmetry rule, stability towards oxidation and reduction of various species in ethene system, propenyl system and cyclobutadiene system, geometry of cyclobutadiene molecule as predicted by SHM and its Jahn-Teller distortion, aromaticity and Huckel's $(4n + 2)$ π electron rule, and calculation of resonance (stabilizing) energy, bond order and atomic charges of various species in ethene system, propenyl system and cyclobutadiene system, strength of SHM, weakness of SHM (detailed explanation) - basis set is limited to p orbitals (p_z orbitals), it treats only π electrons, and the overlap integrals, Fock matrix elements, electron spin and electron-electron repulsion are not calculated/accounted properly, extended Huckel Method (EHM) - minimal valence basis set, calculation of Fock matrix elements, and calculation of overlap integrals by Lowdin orthogonalization, EHM procedure, EHM calculation on protonated helium molecule, application of EHM - an overall idea, strength and weakness of EHM, SCF SE methods - Pariser-Parr-Pople (PPP) method and Complete Neglect of Differential Overlap (CNDO) method - basic principle (an exhaustive treatment is **not** expected).

Unit 5 Density Functional Theory and ab initio Method

(An exhaustive treatment is **not** expected)

Introduction to Density Functional theory and calculations, Kohn-Sham approach - the first and the second Hohenberg-Kohn theorems, introduction to ab initio method and calculation, basis sets for H, He and first, second and third row elements used in ab initio calculations - STO-3G, 3-21G, 3-21G**(*)** and 6-31G*****, these basis sets for a few molecular species (water, methane and carbene), basic principles of ab initio method (an idea only).

TEXT BOOK

1. Computational Chemistry-Introduction to the Theory and Applications of Molecular and Quantum Mechanics - Errol Lewars

22CHY643 Sustainable Chemical Science 3 0 0 3

Evaluation Pattern:

Assessment	Internal	External
Periodical 1 (P1)	15	

Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	
End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1 Green Chemistry and Sustainability

History of green chemistry, chemical composition of the environment (air, water & soil - role of organic and inorganic molecules in pollution), the twelve principles of green chemistry (detailed description with examples), green chemistry as an expression of environmental ethics (Thrift Chemistry), the concept of sustainability, from green to sustainable chemistry, sustainable use of chemical feedstock, water and energy, quantifying greenness of a chemical reaction, green chemistry metrics - mass based, energy and environmental metrics, designing greener process, life cycle assessment (introduction and scope), green toxicology - the need, principles of toxicology, disposition of toxicants in organisms, non-organ system toxicity, mechanistic toxicology, quantitative structure–activity relationships, (environmental toxicology-persistence and bioaccumulation), non-cancer risk assessment, cancer risk assessment, stakeholders in sustainable policy implementation.

Unit 2 Chemistry in water

Definition and attributes of a green solvent, the principle and reasons for use of water in green chemistry-hydrophobicity - cyclodextrin chemistry, Lewis acids in aqueous media, Michael addition in water using triflates, green processes with base in water, green oxidations and reduction in water, on water conditions, use of water in microwave and ultrasonic technology.

Unit 3 Green solvents

Ionic liquids as green solvents - definition and notation - properties, synthesis and use in organic reactions, oxidation, oxidative carbonylation of aniline, Friedel–crafts reaction, Michael addition, Fischer Indole synthesis, benzoin condensation, dimethyl carbonates synthesis in ionic liquids. Super critical fluids- super critical water and carbon dioxide - properties and organic transformations. (Diels Alder, Claisen rearrangement, Fisher Indole, Friedel–crafts reaction, oxidation and hydrogenation. Properties and application in organic transformation of green solvents like polyethylene glycol, glycerol, cyclopentyl methyl ether, 2-methyltetrahydro furan, perfluorinated (fluorous) Solvents - Fluorous Biphase Concept and dimethyl carbonate.

Unit 4 Green Chemistry and Catalysis

Importance of catalysis, turn over number and frequency, the basis of catalysis-kinetic phenomenon, basics of homogeneous, heterogeneous and biocatalysis, Sabatier's principle, catalyst - deactivation, sintering, thermal degradation, inhibition and poisoning, catalyst promoters, modifiers, supported catalysts and reagents for green chemistry- heterogenized reactions for green chemistry, preparation of solid catalyst-slurry and co-precipitation, impregnation, hydrothermal synthesis- drying, calcination, activation and forming, selecting the right support, catalyst characterization- surface characterization methods, temperature programmed techniques, spectroscopy and microscopy. Common mechanism in enzyme catalysis immobilized enzymes, developing biocatalyst- rational design and directed evolution, non-enzymatic biocatalysts.

Unit 5 Green Chemistry Technologies and Alternate Energy Sources

Design for energy efficiency, photochemical reactions, advantages of and challenges faced by photochemical processes (examples). Microwaves as energy source in chemistry - properties of microwaves, microwave heating (effects), approaches to microwave-assisted organic chemistry- solvent free methods, MORE chemistry, continuous microwave reactor (CMR) - microwave batch reactor (MBR), examples of organic transformations. Sonochemistry and Green Chemistry - theoretical basis- cavitation inception, nucleation-bubble dynamics- examples of organic transformations, sono-chemical synthesis of nano-structured materials, electrochemical synthesis- materials manufactured using the process, organic

electrosynthesis- 3-bromothiophen from thiophene. Renewable sources of energy, solar energy, wind power, geothermal solution, hydropower (sources, merits and difficulties in widespread applications), Indian energy scenario- energy conservation act (2001)- features.

REFERENCES

1. *Green chemistry and engineering A Pathway to Sustainability, Anne E. Marteel-Parrish, Martin A. Abraham, American Institute of Chemical Engineers, Inc, John Wiley & Sons, Inc 2014.*
2. *Synthetic organic Sonochemistry, Jean-Louis luche, Springer Science Business Media New York, 1998*
3. *New Methodologies and Techniques for a Sustainable Organic Chemistry, Alessandro Mordini and FerencFaigl, Springer, 2008.*
4. *Green chemistry, Fundamentals and Applications, Suresh C. Ameta and Rakshit Ameta, CRC press, Taylor & Francis Group, 2013*
5. *Handbook of Green Chemistry, Vol5 Green Solvents- Reactions in Water, PualT Anastas, Chao Jun Li*
6. *Sonochemistry: theory, reactions, syntheses, and applications, Filip M. Nowak, Nova Science Publishers, Inc, 2010.*
7. *Green Chemistry Metrics, A Guide to Determining and Evaluating506 Process Greenness, Dicks, Andrew,Hent, Andrei, Springer Briefs in Green Chemistry for Sustainability, 2015*
8. *Catalysis: concepts and applications, Gadi Rothenberg, Wiley-VCH Verlag& Co. KGaA, Weinheim, Germany, 2008*

22CHY644 Sustainable Techniques in Chemical Sciences 3 0 0 3

Evaluation Pattern:

Assessment	Internal	External
Periodical 1 (P1)	15	
Periodical 2 (P2)	15	
Continuous Assessment (CA)*	20	
End Semester		50
Total	**100**	

*CA – Based on Quizzes, Assignments, Projects and Seminars.

Unit 1 From Industrial to Sustainable Chemistry

Industrial Sustainable Chemistry- Managing Intraorganizational Sustainability, Managing Horizontal Interorganizational Sustainability, Managing Vertical Interorganizational Sustainability. Integrated Pollution Prevention and Control- Best Available Techniques reference documents (BREFs), From Industrial Emissions Directive (IED) to Voluntary Systems, Policy Drivers for Sustainable Chemistry (Transition Concept), Development of a CSR Management System Framework. Sustainability Assessment Methods and Tools- Sustainability Assessment Framework, Impact Indicators and Assessment Methodologies, Environmental Impact Assessment, Economic Impact Assessment, Social Impact Indicators, Understanding Industrial Symbiosis-Cluster Management. Sustainability of Logistics in the Chemical Sector, Basic Principles of Chemical Leasing (ChL), Differences between Chemical Leasing and Other Alternative Business Models for Chemicals, Sustainable Chemical Warehousing- Risk Management in the Chemical Warehouse, F^3-Factory concept, Indian energy security scenarios (IESS) 2047.

Unit 2 Process Intensification I

Opportunities and Perspectives for a Sustainable Process Design Definition and Concept, Reaction Engineering, Mixing Principles, Transport Processes, Enhanced Transport Processes, Integrating Process Steps. Moving from Batch to Continuous Processing, Spinning Disc Reactor (Design, Operating Features and Characteristics of SDRs- Green Synthesis of Nanoparticles using SDR), Micro Process Technology- Transport Intensification, Chemical Intensification, Process Design Intensification. Oscillatory Baffled Reactors- Design and operations. Monolith Reactors for Intensified Processing- Design, Hydrodynamics, Advantages and Applications- Cleaner Production of Fuels and Removal of Toxic Emissions. Cavitational Reactors, Mechanism, Reactor Configurations, Transesterification of Vegetable Oils Using Alcohol using Cavitation

Unit 2 Process Intensification II

Membrane Technology- Definitions, functions and operations, biocatalytic membrane reactors (Entrapment, Gelification and Chemical Attachment), biofuel production using enzymatic transesterification. Membrane technology in metal ion removal from waste water, membrane operations for the production of optically pure enantiomers, integrated membrane processes for water desalination. reactive distillation technology and reactive extraction technology- principles, control design and applications. Reactive absorption technology in carbon dioxide capture, removal of nitrogen oxides, desulfurization, and in sulphuric and nitric acid production

Unit 4 Computer Applications in Catalytic Research

Computers as research tools in catalysis- a brief overview, a short over view of modelling methods, data-mining methods in catalysis (PCA, PLS and Artificial Neural networks)

Unit 5 Successful Example of Sustainable Industrial Chemistry

Detailed Process Chemistry of the current technologies and routes for the following chemicals in industry. Industrial Propene Oxide Production (CHPO (Chlorohydrin) Technology, PO/TBA Technology, PO/SM Technology, PO-only Routes). Synthesis of Adipic Acid (Current Technologies for AA Production- Two-Step Transformation of Cyclohexane, Alternatives for AA Production). Ecofining - New Process for Green Diesel Production from Vegetable Oil. Direct Oxidation of Benzene to Phenol, Friedel–Crafts Acylation of Aromatic Ethers Using Zeolites, Sustainable Chemistry in the Production of Nicotinates. Homogeneous catalysis: The Shell higher olefin process (SHOP) and Du Pont synthesis of Adiponitrile. Heterogeneous catalysis: The BP AVADA ethyl acetate process

REFERENCES

1. *Management Principles of Sustainable Industrial Chemistry, Genserik L.L. Reniers, Kenneth Sorensen, and Karl Vrancken (Eds), Wiley-VCH Verlag & Co. KGaA, Boschstr. 12, 69469 Weinheim, Germany, 2013*
2. *Sustainable Development in Practice, Azapagic, A., Perdan, S. (eds.), Wiley-VCH Verlag& Co. KGaA, Boschstr. 12, 69469 Weinheim, Germany, 2011*
3. *The Art of Process Chemistry, Yasuda, N. (ed.), Wiley-VCH Verlag& Co. KGaA, Boschstr. 12, 69469 Weinheim, Germany, 2011*
4. *Sustainable Industrial Chemistry, Centi, G., Trifiro, F., Perathoner, S., Cavani, F. (eds.), Wiley-VCH Verlag& Co. K GaA, Boschstr. 12, 69469 Weinheim, Germany, 2009*
5. *Green chemistry, Fundamentals and Applications, Suresh C. Ameta and RakshitAmeta, CRC Press, Apple Academic Press, Inc, Taylor & Francis Group, 2013*
6. *Catalysis: concepts and applications, Gadi Rothenberg, Wiley-VCH Verlag& Co. KGaA, Weinheim, Germany, 2008*