B.S. in Engineering Chemistry
Department of Chemistry

1. Introduction:

The vision of the Department of Chemistry is to achieve academic excellence and to be recognized for high-quality fundamental, sustainable, and translational research in the chemical sciences and related fields that address ongoing global issues such as energy, food, water, and healthcare. To this end, the department offers a four-year Bachelor of Science (BS) in Engineering Chemistry, aiming to attract young, aspiring minds driven by curiosity and interested in advanced research in academia and industries. The core theme of this undergraduate program is to bridge the gap between fundamental science and engineering, transcending traditional boundaries, and establish ourselves as a leading department at the intersection of science and technology. This distinctive program aligns with the National Education Policy and the Institute's vision of the holistic development of students.

This program is designed to transmit fundamental knowledge in basic science and engineering during the first two semesters, which develops critical analytical thinking and forms the basis of diverse skill sets used by scientists and engineers to innovate, design, and develop technologies for current needs. Students undergo comprehensive training in advanced concepts of chemistry for the next two years. The final year of the curriculum is designed to have flexibility in opting for different courses within the department and across the institute. During this year, the students also get practical experience of the original research being carried out within the department. Industry-Academia Summer Internship, embedded within the curriculum, will ensure hands-on experience in cutting-edge research being pursued in different domains of science and technology. Emphasis is given to the emerging areas in Chemistry to meet societal and industrial needs, and ever-growing sustainability demands. The graduating students of this program shall be equipped with the requisite skill sets required to assume leadership positions in the different sectors of industry, further their career in higher studies, or embark on entrepreneurial ventures to address present-day unmet challenges.

2. Name of the Degree to be Awarded:

B.S. in Engineering Chemistry

3. Objectives of the program

The objectives of this program are:

- To impart education towards understanding of the concepts of chemical science, basic engineering, and allied areas, enabling the students to tackle societal problems through an interdisciplinary approach.
- To equip new generation aspiring minds with chemical science skill-sets founded on engineering aspects, enabling them to opt for challenging career paths at various levels of academia and industry.
- To integrate analytical and computational abilities with experimental skills to create individuals competent in science and innovation practices.
- To facilitate and promote a variety of career paths, including research at an early stage, through capability-linked courses of their choice and academia-industry internships.

- To inculcate an attitude towards commitment to scientific ethics, leadership qualities, entrepreneurship, and professional development for the future generation.

4. Graduate Attributes and Learning Outcomes:

4.1 Graduate Attributes:

- Strong understanding of fundamentals of science and engineering with emphasis on Chemistry.
- In-depth knowledge of the analytical, experimental, and computational methods to study various aspects of engineering in chemistry.
- Foundations for critical thinking that are needed to broaden their careers in diverse cross-disciplines.
- Ability to acquire new knowledge, integrate into the existing paradigm, and innovate solutions to current needs.
- Capability to appreciate synthetic methods for the development of important sustainable chemical products such as pharmaceuticals, agrochemicals, paints, petrochemicals, food additives, plastics, etc.
- Ability to handle analytical, spectroscopic, microscopic and other instrumentation methods for interdisciplinary research areas.
- Use of computational tools to understand and analyse chemical and biophysical processes, molecular structures and advanced materials.
- Writing and presenting scientific articles and technical reports while engaging in ethical and responsible practices for professional growth.

4.2 Learning Outcomes

- Acquire strong fundamentals in theoretical and practical aspects of organic, inorganic and physical and computational chemistry, as well as other branches of basic sciences and engineering.
- Apply the concepts of science and basic engineering to design and analyse novel materials having potential applications to society.
- Develop skills in hands-on wet chemistry, analytical, instrumentation, and experimental data handling to tackle scientific problems.
- Develop communication skills by participating in classroom presentations, seminars and workshops on scientific writing and presentation skills.
- Value of teamwork and group discussion in problem solving, and time management to continue co-curricular activities without compromising academics.
- To understand professional ethics and social responsibilities.

5. Eligibility Criteria & Admission Process:

Admissions to B.S. Programs are made once a year (in July) through the all-India level Joint Entrance Examination (JEE) conducted by IITs. The procedures and other requirements for admission are specified in the JEE Information Brochure brought out every year.

The students will be equipped with skill sets for diverse career perspectives, including roles in chemical industries, pharmaceuticals, petrochemicals, environmental management, and research and development.

6. Expected Outcomes and Impact:

This program will allow graduate students to opt for higher studies, employment in different sectors of industry, entrepreneurship in chemical sciences, and their allied areas. The proposed program, founded on fundamental engineering and advanced chemical science knowledge, is expected to produce graduates with the capability to address real-world challenges related to health care, energy, food, water and environment.

7. Program Structure:

Program Compulsory (PC)	19 Theory & 3 Labs	**66 Credits**
Program Elective (PE)	6	**18 Credits**
Open Elective (OE)	4	**12 Credits**
Project (PP)	2	**6 Credits**
Institute Course		**39 credits**
Total of Non-Graded Courses: Humanities (NH) Engineering (NE)		**6 Credits**
Non-Graded Summer Internship Design Credits		**4 Credit** **2 Credits**
	Total	**153 Credits**

Semester wise plan for BS in Engineering Chemistry

Cat	*Course*	*LTP*	*CH*	*NC*	*GC*	*Cat*	*Course*	*LTP*	*CH*	*NC*	*GC*
	I Semester						**II Semester**				
IE	Engineering Mechanics	3-0-0	3	-	3	IE	Introduction to Machine Learning	3-0-2	5	-	4
IE	Introduction to Computer Science	3-0-2	5	-	4	IS	Chemistry	3-0-0	3	-	3
IS	Physics	3-0-0	3	-	3	IS	Introduction to Bioengineering	2-0-2	4	-	3
IH	HSS I	3-0-0	3		3	IS	Chemistry Lab	0-0-2	2	-	1
IS	Physics Lab	0-0-2	2	-	1						
IS	Mathematics I	2-1-0	3	-	3	IS	Mathematics II	2-1-0	3	-	3
IE	Engineering Drawing	0-0-2	2	-	1	IE	Engineering Workshop	0-0-2	1	-	1
NE	Engineering Design I	0-0-2	2	1	-	NE	Engineering Design II	0-0-2	2	1	-
NH	Communication Skill I	0-0-2	2	1	-	IH	HSS II	3-0-0	3		3
NH	Social Connect and responsibilities I	0-0-1	1	0.5	-	NE	Intro. To Profession	0-0-1	1	0.5	
NH	Performing Arts I /Sports I	0-0-1	1	0.5	-	NH	Performing Arts II /Sports II	0-0-1	1	0.5	-
	Total			**3**	**18**		**Total**			**2**	**18**
	III Semester						**IV Semester**				
PC	Thermodynamics, Kinetics and Engineering Applications	3-0-0	3	-	3	PC	Chemistry of Engineering Materials	3-0-0	3	-	3
PC	Fundamental Organic Chemistry	3-0-0	3	-	3	PC	Quantum Computing in Chemistry	3-0-0	3	-	3
PC	Quantum Chemistry and Applications	3-0-0	3	-	3	PC	Principles of Spectroscopy	3-0-0	3	-	3
PC	Fundamental Inorganic Chemistry	3-0-0	3	-	3	PC	Entrepreneurship for Chemists	3-0-0	3	-	3
PC	Organic Chemistry Lab	0-0-6	6	-	3	PC	Inorganic Chemistry Lab	0-0-6	6	-	3
IE	Environment and Sustainability	3-0-0	3	-	3	PC	Physical and Computational Chemistry Lab	0-0-6	6	-	3

	Total				**18**		**Total**			**-**	**18**
				Summer Internship				**2 Credits**			
	V Semester						**VI Semester**				
PC	Organic Reactions and Mechanisms	3-0-0	3	-	3	PC	Heterocyclic Compounds and Applications	3-0-0	3	-	3
PC	Physical Organic Chemistry	3-0-0	3	-	3	PC	Industrial Catalysis	3-0-0	3	-	3
PC	Main group and Bioinorganic Chemistry	3-0-0	3	-	3	PC	Statistical Thermodynamics	3-0-0	3	-	3
PC	Coordination and Organometallic Chemistry	3-0-0	3	-	3	PC	Solid State and Materials Chemistry	3-0-0	3	-	3
PC	Numerical Methods and Group Theory	3-0-0	3	-	3	PC	Organic Synthesis	3-0-0	3	-	3
PC	AI/ML in Chemistry	3-0-0	3	-	3	PE	Program Elective-2	3-0-0	3	-	3
NH	Professional Ethics I	1-0-0	1	1	-						
PE	Program Elective-1	3-0-0	3	-	3						
	Total			**1**	**21**		**Total**				**18**
			Summer Internship					**2 Credits**			
	VII Semester						**VIII Semester**				
PE	Program Elective- 3	3-0-0	3	-	3	PE	Program Elective-5	3-0-0	3	-	3
PE	Program Elective- 4	3-0-0	3	-	3	PE	Program Elective-6	3-0-0	3	-	3
OE	Open Elective-1	3-0-0	3	-	3	OE	Open Elective-3	3-0-0	3	-	3
OE	Open Elective-2	3-0-0	3	-	3	OE	Open Elective-4	3-0-0	3	-	3
PP	BS Project-1	0-0-3	-	-	3	PP	BS Project-2	0-0-3	-	-	3
	Total		15	-	**15**		**Total**		15	**-**	**15**
											141
									Essential Audit	**12**	**-**
									Grand Total		**153**

Minor in Engineering Chemistry (6 PC)

S.No.	Name	L-T-P
1.	Fundamental Organic Chemistry	3-0-0
2.	Industrial Catalysis	3-0-0
3.	Chemistry of Engineering Materials	3-0-0
4.	Quantum Chemistry and Applications	3-0-0
5.	Quantum Computing in Chemistry	3-0-0
6.	Principles of Spectroscopy	3-0-0

	List of Electives				
S.No.	**Type**	Course name	**L-T-P**	**Credit**	**Level**
1	**PE**	Supramolecular Chemistry and Applications	**3-0-0**	**3**	**600**
2	**PE**	Polymer Material Science	**3-0-0**	**3**	**400**
3	**PE**	Green Chemistry and Applications	**3-0-0**	**3**	**400**
4	**PE**	Organometallic Compounds in Organic Synthesis	**3-0-0**	**3**	**600**
5	**PE**	C–H Bond Activation and Functionalization	**3-0-0**	**3**	**400**
6	**PE**	Chemistry of Organic Biomolecules	**3-0-0**	**3**	**600**
7	**PE**	Nanomaterials and Nanodevices	**3-0-0**	**3**	**600**
8	**PE**	Chemistry of the f-block elements	**3-0-0**	**3**	**600**
9	**PE**	Ligand Design: Principles and Applications	**3-0-0**	**3**	**400**
10	**PE**	Advanced Main Group Chemistry	**3-0-0**	**3**	**600**
11	**PE**	Electrode Materials	**3-0-0**	**3**	**400**
12	**PE**	Water Chemistry	**3-0-0**	**3**	**400**
13	**PE**	Chemical Binding	**3-0-0**	**3**	**600**
14	**PE**	Principles of Fluorescence Spectroscopy and Imaging	**3-0-0**	**3**	**600**
15	**PE**	Single Molecule Spectroscopy	**3-0-0**	**3**	**400**
16	**PE**	Machine Learning for Chemistry	**3-0-0**	**3**	**600**
17	**PE**	Theoretical account of Spectroscopy	**3-0-0**	**3**	**400**
18	**PE**	Principles of Biological Soft Matter	**3-0-0**	**3**	**600**

Course Contents:

Title	**Chemistry**	Course No.	CYL1010
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	B.Tech./ B.S. in Engineering Chemistry	Type	Compulsory
Pre-requisite			

Objective

The instructor will:

1. Relate the fundamental principles of chemistry with practical problems encountered for engineers and place the emphasis on problem-solving
2. Provide knowledge of engineering materials metals, composites, polymers, cement, steel, fuels, batteries and drugs.

Learning Outcomes

Students will be able to:

1. Understanding the behavior of matter and materials using fundamental knowledge of their nature
2. Predict potential complications from combining various chemicals or metals in an engineering setting. (need to change as per external experts)

Contents

Atomic and Molecular Structure: particle in a box, angular momentum, wavefunction, multielectron atoms, homonuclear and heteronuclear diatomic molecules, non-covalent interactions

Electrochemical Systems: Electrochemical cells and EMF, Applications of EMF measurements: Steady state approximation, Chain reactions, photochemical kinetics, Fuel Cells, OER and HER reactions, Corrosion

Surface Chemistry: Surfaces and interfaces, surface modification, surface energy, contact angle and surface tension.

Basic Spectroscopy: Selection Rules, Fundamentals FTIR, Raman, UV-visible, and Fluorescence spectroscopy **(13 Lectures)**

Inorganic Chemistry: Molecular shape, geometry, and molecular symmetry

Solid State Chemistry: Lattice and Unit Cells, Ionic solids, X-Ray Diffraction, Bands in solids, semiconductors, Introduction to nanomaterials. Redox reactions and application in batteries.

Transition Metal Chemistry: Colors in Complexes, Organometallics, Bioinorganic Chemistry (**13 Lectures**)

Organic Chemistry: Application of various organic molecules, such as polymers and biopolymers, drugs, and photoactive molecules in day-to-day life, Organic acid-base chemistry and its applications, Structure and reactivity of hydrocarbons such as alkanes, alkenes, alkynes, and allenes. **(13 Lectures)**

Textbooks

1. Silberberg, M., *Chemistry: The Molecular Nature of Matter and Change*, 6th Edition, McGraw Hill Education.
2. West, A.R., (2015), *Solid State Chemistry and Its Applications*, 2nd edition, John Wiley & Sons.
3. J. D. Lee, Concise Inorganic Chemistry, 5th Edition.
4. Atkins, Physical Chemistry, 11th Edition.

Reference Books

1. McMurry, J. E. & Fay, R. C. *Chemistry*, 5th Edition, Pearson.

2. Hill, R. H. & Finster, D. (2010) *Laboratory Safety for Chemistry Students Laboratory Safety for Chemistry Students,* Wiley.
3. Jonathan Clayden, Nick Greeves, Stuart Warren, Organic Chemistry, 2nd Edition.
4. F. Albert Cotton, Geoffrey Wilkinson, Basic Inorganic Chemistry, Wiley Student Edition.

Online Course Material
https://nptel.ac.in/downloads/122101001/

Title	**Chemistry Lab**	Course No.	CYP1010
Department	Chemistry	L-T-P [C]	0–0–2 [1]
Offered for	BS in Engineering Chemistry/B.Tech.	Type	Compulsory
Prerequisite			

Objectives
The instructor will:
1. Teach basic aspects of spectroscopic methods, important analytical tools in academic and industrial research.
2. Make students aware of laboratory safety and use of hazardous chemicals, importance of material safety data sheets (MSDS).
3. Impart knowledge on the selective techniques of reaction set-up involved in the synthesis.

Learning Outcomes
The students are expected to have the ability to:
1. Determine the structures/functional groups of molecules utilizing several spectroscopic techniques.
2. Understand the basic principles behind the synthesis and properties of compounds.
3. Plan and conduct experiments for synthesis and characterizing molecules.

Contents
Laboratory Experiments:
1. Preparation of Nylon 6,6.
2. Preparation of double salts.
3. Preparation of the salt of Co-ethylenediamine complex.
4. Preparation of tetraphenyl cyclopentadienone by Aldol Condensation.
5. Determination of Critical Micelle Concentration of a Surfactant by Conductivity Method.
6. FTIR spectroscopy in combination with a technique for the analysis of caffeine in tea and coffee.
7. The excitation and emission spectra of Curcumin in solvents ethanol and hexane, respectively, and find the Stokes shift using Fluorescence Spectroscopy.
8. Surface contact angle, surface tension, and surface free energies of different solvents and substrates, respectively.
9. Study of a reversible redox reaction using Cyclic Voltammetric analysis.
10. Study of color in complexes using UV-Visible spectroscopy
11. Determination of enantiomeric purity of Naproxen and Ibuprofen.

Textbook

1. Vogel, A. I., Textbook of Practical Organic

2. Donald L. Pavia, Gary M. Lampman, George S. Kriz, James A. Vyvyan: Introduction to Spectroscopy, 4th Edition, Brookes Cole, 2008.

Self Learning Material

1. http://nptel.ac.in/courses/104103071/26
2. https://ocw.mit.edu/courses/5-37-introduction-to-organic-synthesis-laboratory-spring-2009/pages/labs/

Title	**Thermodynamics, Kinetics and Engineering Applications**	Course No.	CYL2XX0
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	B.S. in Engineering Chemistry	Type	Compulsory
Prerequisite			

Objectives

The instructor will:

1. Delineate fundamental connection of macroscopic thermodynamics and kinetics to microscopic viewpoint through statistical mechanics
2. Detail industry level applications of the concepts borrowed from thermodynamics, equilibrium and reaction kinetics

Learning Outcomes

The students will be able to:

1. Describe thermodynamics, equilibrium and chemical kinetics through a detailed microscopic viewpoint of statistics
2. understand the usage of the fundamental thermodynamic and kinetics concepts in industry level applications namely solubility prediction, refrigeration, controlled solidification, catalysis etc.

Contents

Thermodynamics: Work, heat & energy, Laws of Thermodynamics, Enthalpy, heat capacity, Expansion of ideal gas, Joule-Thomson effect, Linde Refrigerator, changes of enthalpy and entropy of reactions, entropy, spontaneous, irreversible and cyclic processes, Carnot engine and spontaneous cooling in industry, Gibbs-Helmholtz equation, Simple Mixtures and chemical potential, determination of absolute entropies, residual entropy, concept of equilibrium (**9 lectures**)

Types of Equilibrium and applications: Homogeneous and heterogeneous equilibria, equilibrium constant, applicability in Haber-Bosch process, Clausius-Clapeyron equation, Gibbs phase rule, azeotropes, distillation and use in industry, multi-phase equilibria, Eutectic systems and uses in controlling solidification, congruent and incongruent melting and industrial applications, classification of phase transitions, Electrochemical equilibrium, types of cells, Nernst equation and EMF, Types of electrodes, EMFs of electrodes and uses in battery industry(**14 lectures**)

Statistical understanding of Equilibrium and Chemical Kinetics: Macroscopic and microscopic variables, probability, postulates of statistical thermodynamics, ensembles and thermodynamic variables, Partition function, Fluctuations and response functions, Reaction rates, extent and order and molecularity of reactions, Experimental methods to determine order, Arrhenius equation, Collision theory of gaseous reaction, Activated complex theory/Transition State Theory, unimolecular reactions, RRK and RRKM theories, basics of Marcus theory of electron transfer, Fick's law of diffusion, Homogeneous and heterogeneous catalysis, Enzyme catalysis and biophysical applicability, Adsorption on surface, Langmuir isotherm and uses in catalysis, purification in industry, complex reactions, Reaction rates and Partition function (**16 Lectures**)

Textbook

1. Atkins, P.W.; Paula, J.de. (2014), Atkin's Physical Chemistry Ed., 10th Edition, Oxford University Press.
2. Castellan, G. W. (2004), Physical Chemistry, 4th Edition, Narosa.
3. Keith J. Laidler, Chemical Kinetics, Pearson, Third Edition (2003)
4. D. A. McQuarrie and John D Simon, Physical Chemistry, Viva Books, India 2003.

Reference Books

1. D. A. McQuarrie, Statistical Mechanics, University Science Books, 2000
2. B. Bagchi, Statistical Mechanics for Chemistry and Materials Science, CRC press (2018).
3. Molecular Driving Forces: Statistical Thermodynamics in Chemistry and Biology/ by K. A. Dill and
   S. Bromberg, Garland Science, 2003.
4. Molecular Thermodynamics by D. A. McQuarrie, and J. D. Simon, Viva Books, 2018.

Self-Learning Material

1. Basic Thermodynamics, Dr. Suman Chakroborty, NPTEL https://nptel.ac.in/courses/112105123 Sangaranarayanan, M.V., Electrochemistry, Department of Chemistry, IIT Madras; https://nptel.ac.in/courses/104106129
2. Basic Statistical Mechanics, Professor Biman Bagchi, NPTEL, IIT Bombay https://onlinecourses.nptel.ac.in/noc25_cy52/preview

Title	**Fundamental Organic Chemistry**	Course No.	CYL2XX0
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	B.S. in Engineering Chemistry	Type	Compulsory
Pre-requisite			

Objective

The instructor will:

1. Provide insights into the mechanism of a diverse set of organic reactions representing the structures of organic molecules, their active sites, and reactive sites.
2. Provide knowledge of fundamental organic chemistry with regard to efficiency and selectivity of reactions, conformational aspects, and stereochemistry.
3. Provide knowledge of properties, preparations, and reactions for selective classes of molecules

Learning Outcomes

The students are expected to:

1. Understand the reaction pathways and rationale behind drawing a reaction mechanism.
2. Appreciate the crucial role of conformations and configurations in determining the course of organic reactions.
3. Apply the knowledge in predicting reactions and products in organic chemistry.

Contents

Introduction: IUPAC nomenclatures of organic molecules, hybridization, structures, molecular orbitals, concepts of inductive effect, electromeric effect, hyperconjugation, captodative effect **(7 lectures)**.

Basic stereochemistry: Stereoisomerism, Enantiomers, diastereomers, epimers, D/L notations, R/S notations, optical activity, enantiomeric excess, conformational analysis of aliphatic acyclic compounds, angle strain, torsional strain, ring strain, conformation of aliphatic cyclic compounds, such as cyclopropane, cyclobutane, cyclopentane, and cyclohexane **(10 lectures)**.

Reactive Intermediates: Transition states and intermediates, structure and reactivity of carbocations and carbanions (including nonclassical), radicals, carbenes, nitrenes, benzynes **(8 lectures)**.

Identification and characterization: Basics of Infrared Spectroscopy (IR), Nuclear Magnetic Resonance Spectroscopy (NMR), and Mass Spectrometry (MS), stretching frequencies of different organic functional groups, Chemical shifts of different organic functional groups in 1H and 13C NMR, Different ionization techniques (EI, CI, ESI etc.), Fragmentation of organic molecules, Structural elucidation of unknown organic compounds **(9 lectures)**.

Organic Biomolecules: Structure and properties of amino acids, carbohydrates, nucleic acids, lipids, steroids, terpenes, and terpenoids **(5 Lectures)**.

Text Books:

1. Carey, F. A. and Giuliano, R. M., (2012), Organic Chemistry, 8th Edition, McGraw Hill Education
2. Clayden, J., Greeves, N., and Warren, S., (2012), Organic Chemistry, 2nd Edition, Oxford Sykes, P., A Guidebook to Mechanism in Organic Chemistry, 6th Ed., Longman
3. Finar, I. L., Organic Chemistry, Vol 1, The Fundamental Principles, Pearson, Education India

References:

1. Smith, M. B., (2016), March's Advanced Organic Chemistry, 7th Edition. Wiley

Self-learning Material:

1. Punniyamurthy, T., NPTEL Course material, Department of Chemistry, Indian Institute of Technology Guwahati, https://nptel.ac.in/courses/104103022
2. Sunoj, R. B., Organic Reaction Mechanism, NPTEL Course material, Department of Chemistry, Indian Institute of Technology Bombay, http://nptel.ac.in/courses/104101005/

Title	**Fundamental Inorganic Chemistry**	Course No.	CYL2XX0
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	B.S. in Engineering Chemistry	Type	Compulsory
Prerequisite			

Objectives

The Instructor will:

Provide background to basic concepts and key knowledge base of general chemistry and inorganic chemistry to prepare students for careers as professionals in the field of chemistry

Learning Outcomes

The students are expected to have the ability to:

1. Understand the fundamentals of both ionic and covalent compounds, including electronegativities, and predict geometries of simple molecules.
2. The fundamentals of the chemistry of acid-base, and important real-world applications.
3. The basic knowledge about redox processes, nuclear chemistry, and its applications.

Contents

Atomic structure, Multi-electron atoms, Periodic trends. (**7 Lectures**)

VSEPR shapes of small molecules, Symmetry, VBT, Molecular orbital theory: Homo and heteronuclear diatomics, triatomics; Covalent and Ionic solids **(15 Lectures)**

Acid-base chemistry: concepts, measures of acid-base strength, and Hard Soft Acid and Base, acid base chemistry in non-aqueous solvent **(6 Lectures)**

Oxidation and Reduction: oxidation number, reduction potential, half-cell, electrochemical series, Nernst equation, disproportionation reaction, effect of complex formation, precipitation on reduction potential, chemical extraction **(7 Lectures)**

Introduction of nuclear chemistry: Radioactivity, nuclear reactions, half-life, atomic fission, atomic fusion, **(4 Lectures)**

Textbook

1. John E. McMurry, Robert C. Fay (2015), Chemistry, Pearson
2. Lee, J.D. (2012), Concise Inorganic Chemistry, Oxford University Press; 6th edition

Reference Books

1. Inorganic Chemistry: Principles of Structure and Reactivity, 4th Edition, Pearson

Self-Learning Material

1. 1.https://nptel.ac.in/courses/104/101/104101121/
2. https://www.youtube.com/watch?v=0Uj4j6td1es

Title	**Quantum Chemistry and Applications**	Course No.	CYL2XX0
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	B.S. in Engineering Chemistry	Type	Compulsory
Prerequisite	-		

Objectives

The Instructor will:

1. provide an advanced level understanding of quantum chemistry
2. Will show a few applications of quantum mechanics to chemistry

Learning Outcomes

The students are expected to have the ability to:

1. understand quantum mechanics and interpret chemistry problems at the atomistic level
2. apply quantum chemistry to problems in chemistry

Contents

Fundamentals: Old Quantum theory, Correspondence principle, Bohr-Sommerfeld quantization, Wave-particle duality, Stern-Gerlach experiment **(7 Lectures)**

Mathematical Formalism: Operators, Eigenfunctions and eigenvalues, Operators in quantum mechanics, expectation values, Theorems of Quantum Mechanics, Commuting and non-commuting operators, Angular momentum **(8 Lectures)**

Exactly Solvable Problems: Time independent and time dependent wave equation, Particle confined to infinite and finite potential wells, Harmonic oscillator, Rigid rotor, Hydrogen atom **(8 Lectures)**

Approximation Methods: Variational principle, Perturbation theory, Energy and wavefunction corrections **(8 Lectures)**

Quantum Chemistry: Spin, Many-electron problems, Hartree-Fock method, Born-Oppenheimer approximation **(8 Lectures)**

Textbook

3. Quantum Chemistry, I. N. Levine, 7th Edition, PEARSON (2016).

Reference Books

1. Quantum Chemistry, D. A. McQuarrie, Viva Student edition (2016).
2. Modern Quantum Chemistry, A. Szabo and N. S. Ostlund, Dover Books (1996).

Title	**Organic Chemistry Lab**	Number	CYP2XX0
Department	Chemistry	L-T-P [C]	0–0–6 [3]
Offered for	BS in Engineering Chemistry	Type	Compulsory
Prerequisite			

Objectives

The instructor will:

1. Teach basic aspects of isolation and purification techniques, spectroscopic methods, important analytical tools in academic and industrial research.
2. Make students aware of laboratory safety and use of hazardous chemicals, importance of material safety data sheets (MSDS).
3. Impart knowledge on the different techniques of reaction set-up involved in the synthesis.

Learning Outcomes

The students are expected to have the ability to:

1. Determine the structures of known/unknown molecules utilizing several spectroscopic techniques.
2. Understand the basic principles behind the synthesis and properties of compounds.
3. Plan and conduct experiments for synthesis and characterizing molecules.

Contents

Laboratory Experiments:

1. Melting point measurement of a given organic compound
2. Identification of an organic compound by HRMS
3. Identification of functional group present using IR spectroscopy
4. Identification of organic compound using NMR spectroscopy
5. Purification of an organic compounds via recrystallization
6. Separation of mixture of organic molecules by distillation techniques
7. Separation of a mixture of organic compounds by using extraction techniques
8. Chromatography techniques: TLC and Column Chromatography
9. Detection of an organic functional group: aldehyde/ketone
10. Reduction reaction: Reduction of ketone to alcohol
11. Oxidation reaction: Oxidation of primary alcohol to aldehyde using PCC
12. Aromatic electrophilic substitution reaction: Bromination of aniline derivatives
13. Esterification: Synthesis of Aspirin
14. Green Reaction: Reaction in the water medium as a solvent
15. Carbon-Carbon bond formation reaction (Wittig reaction)
16. Protection of functional group (ex. alcohol/amine)

Textbook

1. Robert M. Silverstein, Francis X. Webster, David Kiemle: Spectrometric identification of organic compounds, 7th Edition, Wiley, 2005.
2. G. S. Girolami, T. B. Rauchfuss, R. J. Angelici Synthesis and Technique in Inorganic Chemistry, University Science Books, 3rd Ed, 1999.

Reference Books

1. Harald Gunther: NMR spectroscopy, Basic principles, concepts, and applications in chemistry, 2nd Ed., Wiley, 2001 (reprint)
2. Ault, A., Techniques and Experiments for Organic Chemistry, University Science Books

Self Learning Material

http://nptel.ac.in/courses/104103071/26

Title	**Chemistry of Engineering Materials**	Course No.	CYL2XX0
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	B.S. in Engineering Chemistry	Type	Compulsory
Pre-requisite			

Objective

1. To provide knowledge about structural features, synthesis, and properties of engineering materials.
2. To provide an understanding of the role of chemistry in modern engineering used in materials characterization and their applications.

Learning Outcomes

The students are expected to:

1. Explain structure, synthesis, and structure–property relationships of various material classes.
2. Apply chemical principles and characterization techniques to analyze materials for engineering applications.

Contents

Introduction to Material Chemistry: Classification of engineering materials, structure–property relationships, chemical bonding in materials (ionic, covalent, metallic bonding), crystal structures in materials, defects in solids and their influence on material properties **(4 Lectures)**.

Metallic Materials: Structure and properties of metals, alloys and alloy design, ferrous materials (steel, cast iron), non-ferrous metals (Al, Cu, Ti alloys), heat treatment and strengthening mechanisms, applications in engineering and construction **(4 Lectures)**.

Nanomaterials: Introduction to nanoscale materials, classification, quantum confinement, size-dependent properties, synthesis and applications of nanomaterials and nanocomposites **(6 Lectures)**.

Corrosion and Corrosion Protection: introduction to corrosion, types of corrosion: galvanic, pitting, stress corrosion, factors affecting corrosion, corrosion prevention methods: coatings, cathodic protection. **(2 Lectures)**.

Characterization techniques: Microscopy (SEM, TEM, AFM), spectroscopy (XRD, XPS), Dynamic Light Scattering **(3 Lectures).**

Polymers: Polymerization (addition, condensation), plastics (thermoplastics, thermosets), Advantages of plastics over traditional materials (Wood and Metal), Reinforced or filled plastics: Definition, Advantages, Applications, Polymers in Surgery, Biomedical uses of Polyurethane, PVC, Polypropylene, and Polyethylene. Rubber processing and vulcanization, Composite materials: Definition, Examples, Advantages over metals and polymers, applications (OLEDs), *Lubricants and Adhesives:* types and characteristics, adhesives: natural and synthetic types with applications **(12 Lectures)**.

Materials for Energy and Environment: Materials for batteries and supercapacitors, Fuel cell materials, Hydrogen storage materials, Photocatalytic materials for environmental remediation, Sustainable and green materials, Artificial leaf **(6 Lectures)**.

Characterization techniques for polymers: Solid state NMR, FTIR, and thermal analysis (TGA, DSC) **(2 Lectures)**.

Text Books:

1. Textbook of Nanoscience and Nanotechnology, Murty, Shankar, B Raj, Rath, Murday, Springer (2013)
2. Textbook of Engineering Chemistry, 4th Edition, R Gopalan, D Venkappayya, S Nagarajan, Vikas Publishing House

References:

1. An Introduction to Materials Science & Engineering, W.D. Callister, John Wiley & Sons (2007).
2. Materials Science and Engineering, V. Raghavan, Prentice-Hall of India Private Limited (2003).
3. Chemistry of nanomaterials: Synthesis, properties and applications C. N. R. Rao, Achim Muller, A. K Cheetham, Wiley-VCH, 2004.

Title	**Quantum Computing in Chemistry**	Course No.	CYL2XX0
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	B.S. in Engineering Chemistry	Type	Compulsory
Prerequisite			

Objectives

1. To provide fundamental knowledge and develop a rigorous understanding of how quantum computing algorithms can be applied to solve electronic structure problems in chemistry
2. To focus on VQE-based methods, chemical Hamiltonians, and their practical implementation using modern quantum software such as Qiskit and PennyLane.

Learning Outcomes

The students are expected to have the ability to:

1. Formulate electronic structure problems in a form suitable for quantum computation.
2. Solve computational chemistry problems using fundamentals of quantum computing

Contents

Quantum Chemistry: Many-electron problems, Spin and Spin-statistics theorem; Variational and perturbation theories; Hartree-Fock method; Slater determinants; Basis sets; Molecular Hamiltonian; Born-Oppenheimer approximation; Potential energy surface; H_2^+ ion; Molecular Orbital and Valence Bond theory; Electron correlation; Electronic structure methods (**15 Lectures**)

Quantum Computing Fundamentals: Qubits and quantum states; Bloch sphere representation; quantum gates (single- and multi-qubit); quantum circuits and circuit model; tensor products and multi-qubit systems; superposition and entanglement; measurement theory and expectation values; noise and decoherence; introduction to Qiskit and PennyLane; basic circuit simulation and execution (**8 Lectures**)

Mapping Chemistry to Qubits: Structure of electronic Hamiltonian; one- and two-electron integrals; fermion-to-qubit mappings (Jordan–Wigner and Bravyi–Kitaev transformations); Pauli operator representation of Hamiltonians; decomposition into Pauli strings; measurement of observables and expectation values; Hamiltonian simplification and tapering; illustrative example of H_2 molecule mapping to qubit Hamiltonian (**8 Lectures**)

Applications: Hybrid quantum-classical algorithms; Variational Quantum Eigensolver (VQE); VQE workflow and quantum-classical optimization loop; ansatz design (hardware-efficient and Unitary Coupled Cluster); VQE circuits and model systems; Adapt-VQE and adaptive ansatz construction; error mitigation strategies; Variational quantum deflation (VQD) for excited states properties (**8 Lectures**)

Textbook

1. Quantum Chemistry, I. N. Levine, 7th Edition, PEARSON (2016).
2. Quantum Computation and Quantum Information, M. A. Nielsen and I. L. Chuang, Cambridge University Press (2010).

Reference Books

1. Quantum Chemistry, D. A. McQuarrie, Viva Student edition (2016).
2. Quantum Information and Computation for Chemistry, Sabre Kais, Wiley (2014).

Title	**Principles of Spectroscopy**	Course No.	CYL2XX0
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	B.S. in Engineering Chemistry	Type	Compulsory
Prerequisite			

Objectives

The Instructor will:

1. Introduce a few spectroscopic methods used as analytical techniques in various fields of science and engineering.
2. Provide conceptual background of these methods along with their instrumentation and some applications.

Learning Outcomes

The students are expected to have the ability to:

1. Understand the conceptual background of various spectroscopic techniques
2. Connect quantum mechanics and spectroscopy to interpret experimental findings in research.

Contents

Fundamentals: Electromagnetic radiation, Maxwell's equations, Time-dependent perturbation theory, Interaction of radiation with matter, Intensity of a Transition - Transition Dipole Moment, Fermi's golden rule; Einstein treatment, Lasers and line shapes and line broadening, Laser spectroscopy; Spectroscopic Timescales, Selection rule for photon-molecule interaction, Continuous wave and Fourier Transform spectroscopy, Sensitivity and resolution of spectrum, Instrumentation, Dispersive spectrometers, Fourier Transform spectrometers (**10 Lectures**)

Rotational Spectroscopy: Linear Motion and Rotational Motion, Diatomic Rigid Rotor, Derivation of selection rules for microwave spectra, Isotope effect, Degeneracy, Intensity of Rotational Lines, Non-Rigid Rotor, Polyatomic Molecules, Rotational Raman Spectroscopy (**5 Lectures**)

Vibrational Spectroscopy: Simple harmonic oscillator, Selection rules, Anharmonicity and its effects, Rotational-vibrational spectra, Normal modes of Vibration, FT-IR Spectroscopy, Vibrational Raman spectroscopy (**7 Lectures**)

Electronic spectroscopy: Basic principle, Symmetry and Term Symbols, Born-Oppenheimer approximation, vibrational coarse and rotational fine structures, Vibrational Progression, Pre-dissociation, Selection rules from transition moment integral – Spin selection, Laporte selection, Frank-Condon principle. Jablonski diagram, various photophysical processes, quantum yield expression, Chromophores, Types of electronic transition, Effect of conjugation and solvent. Introduction to photoelectron spectroscopy. (**8 Lectures**)

Magnetic resonance Spectroscopy: Origin of spin and magnetic moment, Zeeman splitting and gyromagnetic ratio, Electron and nuclear spin resonance, Instrumentation, NMR chemical shift and spin-spin coupling, introduction to AB, AX, AMX spin system, 1D 1H and 13 NMR experiments, Pulse sequences; Methods of relaxation, Double resonance techniques; EPR – Instrumentation, First Derivative Spectra, Electron-nuclear hyperfine interaction, theory of first order EPR spectra, analysis of 1st Order spectra, example of EPR spectra of organic radicals and transition metal complexes. (**9 Lectures**)

Textbook

1. Banwell, C. N., (1994), Fundamentals of Molecular Spectroscopy, 3rd Edition, Tata McGraw-Hill
2. Book Company.

3. Bernath, P. F., (2005), Spectra of Atoms and Molecules, 2nd Edition, Oxford University Press
4. J. M. Hollas, Modern Spectroscopy, Wiley India Exclusive, 2015

Reference Books

1. Gunther, H., (1995), NMR Spectroscopy, 2nd Edition, Wiley
2. Atkin's Physical Chemistry., Peter Atkins, Julio De Paula, 7 th Edition, Oxford (2022).
3. William T. Silvast, Laser Fundamentals, Cambridge University Press.

Title	**Entrepreneurship for Chemists**	Course No.	CYL2XX0
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	B.S. in Engineering Chemistry	Type	Compulsory
Pre-requisite			

Objective

The course aims to:
1. Introduce students to intellectual property protection and innovation in chemical sciences
2. Develop the ability to identify commercial opportunities from chemical research
3. Expose students to startup ecosystems, funding mechanisms, and business models

Learning Outcomes

Students will be able to:
1. Explain the fundamentals of entrepreneurship and innovation in the chemical industries
2. Identify commercial opportunities arising from chemical research and technologies
3. Understand intellectual property protection and patenting strategies for chemical inventions
4. Develop business models and present a technology-based startup idea or commercialization plan

Contents

Introduction to Entrepreneurship: Role of entrepreneurship in economic development, entrepreneurship in chemical industries, academic entrepreneurship and technology transfer **(4 Lectures)**.

Innovation in Chemical Sciences: Idea generation and design thinking, identifying industrial problems in chemistry, translating chemistry research into products, market opportunity assessment, feasibility analysis, Technology Readiness Levels (TRL), innovation pathways in pharmaceuticals, catalysis, materials, case studies of chemical startups **(8 Lectures)**.

Intellectual Property and Business Models: Types of intellectual property, patents in chemical sciences, patent searching and prior art analysis, technology transfer and licensing, business model canvas in chemical and pharmaceutical industries, customer discovery and pricing strategies **(7 Lectures)**.

Product Commercialization and Startup Financing: Lab-to-market translation, process scale-up, regulatory frameworks, funding sources, venture capital and angel investment, government funding schemes, and financial planning **(7 Lectures)**.

Go-To-Market Strategies and Startup Management: Market analysis, competitive landscape, marketing strategies for chemical products, strategic partnerships, team building and leadership, operations in chemical companies, risk management **(4 Lectures)**.

Case Studies and Future Opportunities: Successful chemistry startups, green chemistry entrepreneurship, AI and digital technologies in chemical innovation, student startup pitch presentations, future career paths in entrepreneurship **(9 Lectures)**.

Text Books:

1. J. García-Martínez, K. Li, (2022), *Chemistry Entrepreneurship*, Wiley-VCH GmbH.
2. J. Leker, C. Gelhard, S. von Delft, (2018), *Business Chemistry: How to Build and Sustain Thriving Businesses in the Chemical Industry*, Wiley.

References:

1. E. Ries, (2011), *The Lean Startup,* Portfolio Penguin (Penguin Group).
2. P. Thiel, (2014), *Zero to One*, Crown Business / Crown Currency.

Title	**Inorganic Chemistry Lab**	Course No.	CYP2XX0
Department	Chemistry	L-T-P [C]	0–0–6 [3]
Offered for	B.S. in Engineering Chemistry	Type	Compulsory
Prerequisite			

Objectives
The instructor will:
1. Impart knowledge on the different techniques of reaction set-up involved in the synthesis, isolation, and purification of organic and inorganic compounds.
2. Provide hands-on experience with diverse spectroscopic characterization techniques.

Learning Outcomes
The students are expected to have the ability to:
1. Learn basic experimental techniques in inorganic chemistry
2. Understand the basic principles behind the synthesis and properties of inorganic compounds.
3. Plan and conduct experiments for synthesis and characterizing inorganic compounds.

Contents
Laboratory Experiments:
1. Preparation of nitro- and nitrito-pentamminecobalt(III) chloride
2. Aquation of trans-dichloro-bis(1,2-diamminoethane)cobalt(III)chloride
3. The Preparation and resolution of tris(ethylenediamine)cobalt(III)ion into its optical antipodes
4. Synthesis and reactions of organocobaloximes
5. Synthesis and characterization of RuHCl(CO)(PPh3)3 Introduction to organometallic synthesis under inert atmosphere.
6. Preparation of TiO2 from Titanium Isopropoxide
7. Preparation and Characterization of Hydroxyapatite
8. Preparation and magnetic properties of Fe(III)(acac) complex
9. FLP H_2 activation and hydrogenation reactions
10. Synthesis and characterization of bispyridine iodide nitrate
11. The preparation of pentammineaquocobalt(III) chloride
12. Solid phase Synthesis and characterization of trans bis glycinato Cu(II)
13. The preparation of two crystalline binary transition metal p-toluenesulfonate salts of $[MII(OH2)_6]$- $[OTs]_2$ stoichiometry, Where, MII = Co (1) and Ni (2).
14. Synthesis and characterization of $NiCl_2(PPh_3)_2$ complex
15. Color effects due to ligand-exchange in nickel complexes (Influence of ligand field tetragonality on the ground state spin of nickel (II) complexes with NH_3 and H_2O and ethylene diamine.)
16. Color effects in aqueous systems containing divalent 3d metal ions
17. The preparation of cis-and trans -potassiumdioxalatodiaquochromate(III)
18. Synthesis and characterization of acetylferrocene from ferrocene

Textbook

1. Vogel, A. I., Textbook of Practical Organic
2. G. S. Girolami, T. B. Rauchfuss, R. J. Angelici Synthesis and Technique in Inorganic Chemistry, University Science Books, 3rd Ed, 1999.
3. Elias, A. J., A Collection of Interesting General Chemistry Experiments, Universities Press(India) Pvt. Ltd., 2002

Reference Books

1. J. Derek Woolins, Inorganic Experiments, 3rd Edition, Wiley, 2010.
2. Roesky, H. W.; Muckel, K., Chemical Curiosities: spectacular experiments and inspired quotes, VCH, 1996.

Self-Learning Material

1. http://nptel.ac.in/courses/104103071/26
2. John Dolhun. 5.301 Chemistry Laboratory Techniques. January IAP 2012. Massachusetts Institute of Technology: MIT Open Courseware, https://ocw.mit.edu.

Title	**Physical and Computational Chemistry Lab**	Course No.	CYP2XX0
Department	Chemistry	L-T-P [C]	0–0–6 [3]
Offered for	B.S. in Engineering Chemistry	Type	Compulsory
Prerequisite			

Objectives

The Instructor(s) will:

1. Connect the basic principles of physical chemistry with experiments.
2. Enable students to apply theoretical understandings of various concepts to analytical techniques.
3. Provide knowledge of electronic structure calculations and molecular dynamics simulations

Learning Outcomes

The students are expected to have the ability to:

1. Design, execute and analyse experiments and their outcome.
2. Operate various analytical instruments available in the Institute.
3. Perform electronic structure calculations and molecular dynamics simulations

Contents

pH-metry: (i) Determination of pK_a values of weak monobasic, dibasic, and polybasic acids by pH-metric method (e.g., using acetic acid, succinic acid, oxalic acid, and phosphoric acid, etc.). (ii) Determination of phosphoric acid content in soft drinks: Use of pH sensor and titrimetric analysis

Kinetics: (i) Determination of rate constant for first-order acid-catalysed hydrolysis of an ester (V_0 and V∝ be supplied). (ii) Determination of the rate constant of decomposition of H_2O_2 by acidified KI solution using a clock reaction. (iii) Determination of the equilibrium constant of the reaction KI + I_2 KI_3 by the partition method (partition coefficient to be supplied).

Electrochemistry: (i) Determination of E_0 of Fe^{+3}/Fe^{+2} couples in hydrogen scale by potentiometric titration of ferrous ammonium sulfate solution using $KMnO_4$ or $K_2Cr_2O_7$ as standard.

Titration: (i) Estimation of sodium carbonate using standardized HCl. (ii) Estimation of carbonate and hydroxide present together in a mixture. (iii) Estimation of carbonate and bicarbonate present together in a mixture. (iv) Estimation of free alkali present in different soaps/detergents.

Spectroscopy: (i) Determination of complex concentration using Beer-Lambert's law (ii) Determination of molar extinction coefficient using Beer-Lambert's law (iii) Identification of functional groups using FTIR spectra of some well-known laboratory compounds. (iv) Determination of concentration of caffeine in soft drinks using FTIR

Computational Lab: Drawing geometry of molecules; Single-point energy calculations; Geometry optimization; Equilibrium and Saddle points; HF and DFT calculations ; Build bonded and non-bonded potential parameters after geometry optimization, Energy minimization of a bulk system at meso-scale, VMD, Run molecular simulation in ensemble

Textbook

1. Khosla, B.D.; Garg, V.C.; Gulati, A. (2015),Senior Practical Physical Chemistry, R. Chand & Co, New Delhi
2. Kapoor, K.L. (2019),A Textbook of Physical Chemistry, Vol.7, 1st Edition, McGraw Hill Education.
3. Garland, C. W.; Nibler, J. W.; Shoemaker, D. P.(2003),Experiments in Physical Chemistry, 8th Edition, McGraw-Hill, New York.
4. Quantum Chemistry, I. N. Levine, 7th Edition, PEARSON (2016).

5. Leach, A. Molecular Modelling, 2nd Edition, PEARSON (2001).

Reference Books

1. Ghosal, Mahapatra and Nad (2014) – An Advanced Course in Practical Chemistry, New Central Book Agency.

Title	**Organic Reactions and Mechanisms**	Course No.	CYL4XX0
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	B.S. in Engineering Chemistry and M.Sc. Chemistry	Type	Compulsory
Pre-requisite			

Objective

The objective of the course is:

1. To familiarize students with organic reactions and provide deeper insight into the reaction mechanisms.
2. To broaden their understanding of organic chemistry with emphasis on the efficiency and selectivity of organic reactions.

Learning Outcomes

The students are expected to:

1. Be able to propose mechanisms for complex organic reactions.
2. Understand and predict the orbital interactions involved in organic reactions.

Contents

Introduction: Organic Reactions and their mechanisms; methods for determining reaction mechanisms; transition states and reactive intermediates; crossover experiments; molecular orbital interactions in common functional groups **(7 lectures)**.

Acid and base catalysis: The pK_a scale and its interpretation; pK_a of acids; pK_b (pK_aH) of bases; general and specific acid-base catalysis **(3 lectures)**.

Classification of reactions: Substitution, elimination and addition reactions; aromaticity; electrophilic and nucleophilic aromatic substitution reactions **(9 lectures)**.

Selectivity in organic reactions: Chemoselectivity, regioselectivity, enantioselectivity, diastereoselectivity, stereoselectivity, and stereospecificity in organic reactions; chiral pool synthesis **(8 lectures)**.

Radical Chemistry: Free radicals, radical anions, radical cations; radical initiators; radical halogenation of alkanes; Named reactions involving radical intermediates **(5 lectures)**.

Rearrangements and migrations: Cationic and carbanionic rearrangements; carbene and carbenoid-based rearrangements **(7 lectures)**.

Text Books:

1. Sykes,P., (2013), A Guidebook to Mechanism in Organic Chemistry, 6th Edition, Longman
2. Clayden,J., Greeves,N., and Warren,S., (2012), Organic Chemistry, 2nd Edition, Oxford
3. Carey,F.A., and Sundberg,R.J., (2007) Advanced Organic Chemistry, Part A: Structure and Mechanisms, 4th Edition, Plenum

References:

1. Gossman,R.B., (2008), The Art of Writing Reasonable Organic Reaction Mechanism, Springer

Self-learning Material:

1. Sunoj,R.B., Organic Reaction Mechanism, NPTEL Course Material, Department of Chemistry, Indian Institute of Technology Bombay, http://nptel.ac.in/courses/104101005/

Title	**Physical Organic Chemistry**	Course No.	CYL4XX0
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	B.S. in Engineering Chemistry and M.Sc. Chemistry	Type	Compulsory
Pre-requisite			

Objective

The instructor will:

1 To provide physical concepts of organic chemistry
1. To provide knowledge in pericyclic and photochemical reactions

Learning Outcomes

The students are expected to:

1. Be able to understand the course of organic reactions with regard to physical concepts and stereochemical models
2. Develop an in-depth knowledge with mechanistic understanding in pericyclic and photochemical reactions and apply those in the synthesis of organic compounds

Contents

Introduction: Brief review of basic physical organic concepts **(2 lectures)**.

Stereoelectronic Effects: Participation of sigma and pi bonds in transition state, Orbital symmetry and frontier orbitals, Hammond's Postulate, Hammette Plot, Curtin–Hammett principle **(6 lectures)**.

Stereochemical Models: Cram Model, Felkin-Anh Model, Chelation Model, Prelog's Model Zimmerman-Traxler Model **(7 lectures)**.

Pericyclic Reactions: Introduction of pericyclic reactions, Classifications, Cycloaddition, Electrocyclic, Sigmatropic, Group transfer reactions **(14 lectures)**.

Photochemistry: Basic principles of photochemistry, Retinal isomerization, Photochemical reaction of cyclic and acyclic carbonyl compounds, including enones and dienones, photochemistry of alkenes, dienes, aromatic compounds **(10 lectures)**.

Text Books:

1. Anslyn, E. V. and Dougherty, D. A., (2006), Modern Physical Organic Chemistry, University Science Books
2. Singh, J. and Singh, J., (2012), Photochemistry and Pericyclic Reactions, 3rd Edition. New Age

References:

1. Smith, M. B., (2016), March's Advanced Organic Chemistry, 7th Edition. Wiley
2. Carey, F. A. and Sundberg, R. J., (2007), Advanced Organic Chemistry Part A: Structure and Mechanisms, 5th Edition. Springer
3. Carey, F. A. and Sundberg, R. J. (2007), Advanced Organic Chemistry Part B: Reactions and Synthesis, 5th Edition. Springer

Self-learning Material:

1. Singh, N.D. P., Organic Chemistry and Pericyclic Reactions, NPTEL Course material, Department of Chemistry, Indian Institute of Technology Kharagpur, http://www.nptel.ac.in/courses/ 104105071/

Title	**Main Group and Bioinorganic Chemistry**	Course No.	CYL4XX0
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	B.S. in Engineering Chemistry and M.Sc. Chemistry	Type	Compulsory
Prerequisite			

Objectives

The Instructor will:

1. Give better insight into chemistry of main group elements and bioinorganic chemistry
2. Provide broad knowledge about properties and applications of compounds of main group elements and metal ions essential in biological systems.

Learning Outcomes

The students are expected to have the ability to:

1. Appreciate chemistry of elements essential in biological systems.
2. Understand structure and bonding concepts in chemistry of s- and p-block elements and systematic understanding of their chemical reactivity

Contents

Chemistry of main group elements: Molecular Geometry and Symmetry, hypervalency, Synthesis, structure and bonding in polyhedral boranes and carboranes, Wade's Rules, Berry Pseudorotation, electron count, Isolobal analogy. B-N, P-N, S-N unit containing compounds. Compounds of Silicon, Zeolites. Hydrides, halides, oxides, nitrides of s- and p- block elements. Allotropes of Carbon, introduction to carbenes and their heavier analogues. Chemistry of halogens and Noble gases, Chemistry of s-block elements. Organometallic compounds of main group elements. (**15 Lectures**)
Spectroscopic Characterization: NMR (Including temperature (VT) NMR, e.g., PF_3Cl_2), FT-IR, Raman, Mass etc. (**4 Lectures**)
Applications of main group compounds: Frustrated Lewis pairs and small molecule activation, Synthetic uses of main group complexes, Oxidizing/reducing agents. Precursors for materials deposition. Maingroup based polymers. Deposition of thin films of materials, with a strong focus on Chemical Vapour Deposition (CVD) and ALD. PET and SPECT imaging. (**8 Lectures**)
Bioinorganic Chemistry: Transition metals in biology - their occurrence and function, active-site structure, Metalloenzymes; O2 binding properties of heme (hemoglobin and myoglobin) and non-heme proteins hemocyanin & hemerythrin), co-operativity effect,

Bohr Effect; representative synthetic models of heme and nonheme systems. Electron transfer proteins - active site structure and functions of ferredoxin, rubredoxin and cytochromes, and their comparisons. Metals in medicine. (**12 Lectures**)

Textbook

1. 1. Huheey, J. E., (2008), *Inorganic Chemistry*, 4th edition, Pearson
2. Housecroft, C. E., and Sharpe, A. G., (2012), *Inorganic Chemistry*, 4th Edition, Pearson
3. Miessler G. L., (2014), *Inorganic Chemistry*, 4th edition, Pearson

Reference Books

1. S. J. Lippard (1994) Principles of Bioinorganic Chemistry, University Science Books.
2. Norman, N. C., (2014), *Periodicity and the p-Block Elements*, Oxford Primer Nos. 51,2nd Edition, Oxford University Press
3. Atkins, P. (2010) *Inorganic Chemistry*, 5th Edition, Oxford University Press

Self Learning Material

1. Balakrishna, M. S., *Chemistry of Main Group Elements*, NPTEL Course Material, Department of Chemistry, Indian Institute of Technology Bombay, http://nptel.ac.in/courses/117101105/
2. Ray, D., *Bioinorganic Chemistry*, NPTEL Course Material, Department of Chemistry, Indian Institute of Technology, Kharagpur, http://nptel.ac.in/courses/104105031/

Title	**Coordination and Organometallic Chemistry**	Course No.	CYL4XX0
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	B.S. in Engineering Chemistry and M.Sc. Chemistry	Type	Compulsory
Prerequisite			

Objectives

The Instructor will:

1. Provide background to basic concepts and key knowledge base of Coordination and Organometallic Chemistry.

Learning Outcomes

The students are expected to have the ability to:

1. Understand the bonding fundamentals for both coordination compounds, predicting geometries of simple molecules.
2. Appreciate the fundamentals of organometallic chemistry.

Contents

Introduction: Coordination geometry, coordination numbers, ligands, isomerism, thermodynamic stability, step-wise and overall binding constant, chelate and macrocyclic effect. (**3 Lectures**)

Theories of Bonding: VBT, CFT, MOT and their limitations; splitting of d-orbitals. Spectral and magnetic properties; Color of complexes, term symbols, selection rules for electronic transitions, Orgel and TS diagram, and Nephelauxetic effect, magnetochemistry, Jahn-Teller theorem. (**11 Lectures**)

Inorganic reactions and mechanisms: Hydrolysis reactions, substitution reactions trans-effect; isomerization reactions; metal-metal bonding, cluster compounds (**5 Lectures**)
Transition metal organometallics: Introduction: various sigma/pi donor acceptor ligands, 18 electron rule isolobal analogie. Metal carbonyls, metal phosphines, olefin and acetylene complexes, alkyls and allyl complexes, metallocenes, carbenes and NHC complexes Major reaction types – oxidative addition, reductive elimination, migratory insertion, elimination isomerization and rearrangement reactions. **(12 Lectures)**
Chemistry of f-block elements: Introduction, Structure and bonding, Shift reagents, strong magnets, Luminescence, Separation and Extraction Techniques. Organometallic compounds of f-block elements: synthesis structure bonding and properties **(5 Lectures)**
Organometallic compounds in medicinal and material chemistry **(3 Lectures)**

Textbook

1. Huheey, J.E. Keiter, E. A.; Keiter, R. L.; Medhi, O.K.; (2006), Inorganic Chemistry, Pearson; 4th edition
2. Cotton, F. A.; Wilkinson, G.; Basic Inorganic Chemistry (2007), Wiley; 3rd edition

Reference Books

1. Housecroft, C and Sharpe, A. G. (2012) Inorganic Chemistry, 4th Edition, Pearson

Self-Learning Material

1. Ray, D Coordination Chemistry, NPTEL course material, Department of Chemistry, Indian Institute of Technology, Kharagpur, http://nptel.ac.in/courses/104105033/
2. Maiti, D., Basics in Inorganic Chemistry, NPTEL Course Material, Department of Chemistry, Indian Institute of Technology, Bombay, https://www.youtube.com/watch?v=0ofu2inFF0k&list

Title	**Numerical Methods and Group Theory**	Course No.	CYL4XX0
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	B.S. in Engineering Chemistry and M.Sc. Chemistry	Type	Compulsory
Prerequisite			

Objectives

1. Basic mathematics and numerical techniques required for Chemistry students
2. Knowledge on error analysis to be used for laboratory courses
3. Provide the fundamentals of group theory to understand structure, chemical bonding and spectroscopy

Learning Outcomes

1. Ability to analyze data and perform error analysis on the data
2. Ability to understand and appreciate the mathematical and group theoretical concepts behind chemical theories

Course Content

Mathematical Concepts: Vectors and Vector spaces, Operators, Orthogonal and Unitary matrices, Diagonalization, Matrix eigenvalue problems, Systems of linear algebraic equations, Determinants, Ordinary and partial differential equations, Fourier and Laplace transformation **(13 Lectures)**
Numerical Methods: Errors in Data, Absolute and relative errors, Distribution of Errors, Central Limit Theorem, Linear regression and correlation, Interpolation, Roots of Equations, Algorithms for Matrix **(13 Lectures)**
Group Theory: Symmetry elements and Point Groups, Group postulates and definitions, Group multiplication tables, Subgroups and cosets, Symmetry classes and conjugates, Reducible and irreducible representations, Representations and character tables, Group theory and quantum mechanics, Group theory and chemical bonding, Applications of group theory to structures and spectroscopy, Group theory and crystal symmetry **(13 Lectures)**

Text Books

1. Kreyszig, E., (2011) *Advanced Engineering Mathematics*, 9th Ed., Wiley
2. Cotton, F. A., (2008) *Chemical Applications of Group Theory*, 3rd Ed., Wiley India

Reference Books:

1. Louis, L., (1991) *A Practical Guide to Data Analysis for Physical Science students*, Cambridge University Press
2. Louis, L., (2005) *Mathematics for Science Students*, Cambridge University Press
3. Arfken, W. and Harris, P. (2012) *Mathematical Methods for Physicists*, 7th Ed., Elsevier
4. Bishop, D. M., (1993), *Group Theory and Chemistry,* 2nd Ed., Dover Publications, New York

Online Course Material:

1. Iyengar, S. R. K., *Numerical Methods and Computation,* NPTEL course material, Department of Mathematics, IIT Delhi
2. https://www.youtube.com/watch?v=88ys5ZIolSg&list=PL6E313980EF23CA6E
3. Chandra, M., *Chemical Applications of Symmetry and Group Theory,* NPTEL course material, Department of Chemistry, IIT Kanpur
4. https://www.youtube.com/watch?v=Av9f25sqLG0&list=PLj_Alq7xw30knZPTp a9whzqiSn_RZHGWP

Title	**AI/ML in Chemistry**	Course No.	CYL3XX0
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	B.S. in Engineering Chemistry	Type	Compulsory
Prerequisite			

Objectives

The objectives of this course are to:

1. Introduce the fundamental concepts of machine learning in the context of chemistry
2. Emphasize conceptual understanding, chemical intuition, and interpretation of machine learning models.

Learning Outcomes

After completing this course, students will be able to:

1. Relate machine learning methods to chemical problems
2. Interpret output of regression and classification models
3. Comprehend machine learning applications in chemistry

Contents:

Basics: Mathematical essentials; Vectors; Matrices; Probability; Linear regression; Optimization; Calculus and graph theory; Artificial Intelligence (AI) and Machine learning (ML) in Chemistry; Review of supervised, unsupervised and Reinforcement learning; Regression Models: linear and polynomial regression, regularization; Classification models; Data in Chemistry: Structures, Energies, and Spectra; Features and representations; Training *vs* testing; Overfitting; Error metrics (RMSE, MAE) (**13 lectures**)
Neural Networks: Biological inspiration; Perceptron; Multilayer neural networks; Bias and weights; Activation functions; Training neural networks (**11 lectures**)
Applications in Chemistry: Molecular representations in computers; Smiles representation; Chemical property selection and feature identification; Molecular descriptors; ML for potential energy surfaces and force fields (**15 lectures**)

Textbook

1. *Machine Learning,* T. M. Mitchell, McGraw Hill Education, 1st Edition, 2017.
2. *Machine Learning in Chemistry: The Impact of Artificial Intelligence,* Hugh M. Cartwright (Ed.), Royal Society of Chemistry, 2020.

References:

1. Introduction to Machine Learning, E. Alpaydin, MIT Press, 2020.
2. Machine Learning in Chemistry; Jon Paul Janet and Heather J. Kulik, American Chemical Society, 2020. DOI: 10.1021/acs.infocus.7e4001

Online Material

1. Introduction to Machine Learning, Prof. Balaraman Ravindran, NPTEL

Title	**Organic Synthesis**	Course No.	CYL4XXX
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	B.S. in Engineering Chemistry and M.Sc. Chemistry	Type	Compulsory
Pre-requisite			

Objective

The instructor will:

1. To provide an understanding of diverse chemical reactions and their application in synthesis
2. To provide knowledge of key aspects of retrosynthesis of simple-to-complex organic molecules.

Learning Outcomes

The students are expected to:

1. Acquire the knowledge and skills required to strategize and plan organic synthesis,
2. Develop an understanding of total synthesis of organic molecules.

Contents

Functional group interconversions and Name reactions: Principles of functional group interconversions; Reactivity patterns of common functional groups; Carbon–carbon and carbon–heteroatom bond-forming reactions; Important name reactions in organic synthesis; Mechanistic aspects and synthetic applications of selected name reactions **(10 lectures)**.

Transition Metal-Catalyzed Reactions in Organic Synthesis: Introduction to organometallic and transition metal chemistry; Transition metal-catalyzed cross-coupling reactions; Palladium-, nickel-, and copper-catalyzed transformations; Fundamental organometallic processes (Oxidative addition, Reductive elimination, Transmetallation, Migratory insertion) Catalytic cycles and mechanistic pathways; Synthetic applications of cross-coupling reactions in modern organic synthesis **(9 lectures)**.

Oxidation and Reduction Reactions in Organic Synthesis: Fundamentals of oxidation and reduction reactions; Oxidation states and redox concepts in organic chemistry; Common oxidizing reagents and their synthetic applications; Common reducing reagents and selective reductions; Chemoselective and stereoselective redox transformations; Name reactions involving oxidation and reduction processes; Applications of redox reactions in multistep organic synthesis **(8 lectures)**.

Carbanions and Organometallic Reagents in Synthesis: Generation, stability, and reactivity of carbanions; Alkylation reactions of enolates; Synthetic applications of enamines and hydrazones; Alkylation of heteroatom-stabilized anions; Organometallic reagents: preparation and properties; Applications of organolithium, Grignard, and related reagents in organic synthesis; Carbon–carbon bond formation using organometallic intermediates **(7 lectures)**.

Strategy and Design in Organic Synthesis: Principles of retrosynthetic analysis; Synthetic planning and disconnection approaches; Concepts of synthetic equivalents; Umpolung and polarity inversion strategies; Design and execution of efficient multistep organic syntheses **(5 lectures)**.

Text Books:

1. Warren,S., and Wyatt.P., (2008), Organic Synthesis: The Disconnection Approach, 2nd Edition, Wiley-VCH
2. Carey,F.A., Sundberg,R.J., (2007), Advanced Organic Chemistry, Part B: Reactions and Synthesis, 5th Edition, Plenum
3. Carruthers, W., (1989), Some Modern Methods in Organic Synthesis, Cambridge
4. Clayden,J., Greeves,N., and Warren,S., (2012) Organic Chemistry, 2nd Ed., Oxford

References:

1. Nicolaou,K.C., Sorensen,E.J., (1996), Classics in Total Synthesis: Targets, Strategies and Methods, 1st Edition, Wiley-VCH

Self-Learning Material

1. Punniyamurthy,T., Principles of Organic Synthesis, NPTEL Course Material, Department of Chemistry, Indian Institute of Technology Guwahati, http://www.nptel.ac.in/courses/104103022/

Title	**Heterocyclic Compounds and Applications**	Course No.	CYL4XX0
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	B.S. in Engineering Chemistry and M.Sc. Chemistry	Type	Compulsory
Pre-requisite			

Objective

The instructor will:

1. Provide insight into the fundamental reactivity and synthesis of heterocycles, and
2. Broaden their knowledge in the field of heterocyclic chemistry with regard to its application in the synthesis of natural products and pharmaceuticals.

Learning Outcomes

Students will be able to:

1. Understand the basic heterocyclic principles and apply different types of organic reactions in the synthesis of small heterocyclic compounds.
2. Learn the applications of modern organic synthetic tools in the efficient synthesis of heterocycles.
3. Design and propose routes for the synthesis of natural products and pharmaceuticals based on heterocycles.

Contents

Introduction: Importance of heterocyclic compounds, Nomenclature of heterocyclic ring systems **(3 lectures)**.

Three-membered Heterocycles: Structure, reactivity and synthesis of Oxirane, Thiirane, and Aziridine **(3 lectures)**.

Four-membered Heterocycles: Structure, reactivity and synthesis of four membered Heterocycles such as Oxetane, Thietane and Azetine **(3 lectures)**.

Five-membered Heterocycles: Structure, reactivity and synthesis of five membered Heterocycles such as Pyrrole and pyrrolidine, Thiophene and tetrahydrothiophene, Furan and tetrahydrofuran, chemistry of Pyrazole, Imidazole, Oxazole, Thiazole **(10 lectures)**.

Six-membered Heterocycles: Structure, reactivity and synthesis of Six membered Heterocycles: Pyridine and Piperidine, pyran and Tetrahydropyran, pyridones, Pyridine-N-oxides **(10 lectures)**.

Polycyclic heterocycles: Structure, reactivity and synthesis of Indole, Quinoline and Isoquinoline, Coumarins and Chromones, benzimidazole and benzoxazole **(6 lectures)**.

Modern Methods: Synthesis of heterocycles using modern sustainable methods **(4 lectures)**.

Text Books:

1. J. A. Joule and K. Mills, Heterocyclic Chemistry, 5th Ed., Wiley, 2010.

References:

1. R. K. Bansal, Heterocyclic Chemistry, 5th Ed., New Age International Private Limited, 2017.

Self-Learning Material

1. NPTEL Lectures : Heterocyclic Chemistry- http://nptel.ac.in/courses/104105034/

Title	**Statistical Thermodynamics**	Course No.	CYL4XX0
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	B.S. in Engineering Chemistry and M.Sc. Chemistry	Type	Compulsory
Prerequisite			

Objectives
The Instructor will:
1. Provide the connection between microscopic theory and thermodynamics.
2. Describe how complex phenomena can be transferred into simple models.

Learning Outcomes
The students are expected to:
1. Predict properties of many-body systems starting from its microscopic constituents and their interactions
2. Connect microscopic theory to chemical reaction

Contents
Mathematical foundation: Probability theory, Permutation and combination, Conditional probability and independent events, Random variables and their probability distribution, Central limit theorem, Binomial distribution, Stirling's approximation, Method of Lagrange multiplier; Statistics of scientific measurement, Error, Maximum likelihood method, Curve fitting, Least square fit; Dirac delta function, Uniform distribution and Dirac delta function, Partial differential equation, equation of continuity (**11 Lectures**)
Statistical thermodynamics: Micro and Macro states, postulates, concepts of distinguishable and indistinguishable particles, Microcanonical Ensemble (NVE), Canonical Ensembles or Isothermal-isochoric (NVT) Ensembles, Isothermal-isobaric (NPT) and Grand Canonical Ensemble (μVT), Equivalence of Ensembles, Boltzmann distribution, Entropy, partition functions for different ensemble, calculations of thermodynamic properties of each of ensemble, ideal monatomic and diatomic gas, Applications of canonical ensemble, 1D Ising model, Ideal and real gas, Sackur Tetrode equation, Phase space, Ergodicity, Liouville's Theorem (**15 Lectures**)
Applications: Fluctuations and thermodynamic properties, Heat capacity, compressibility, Linear response theory, Partition function and Transition State Theory, classical fluids, Pair correlation functions, Response functions, Langevin Equation, Fluctuation-Dissipation Theorem, Diffusion (**13 Lectures**)

Textbook
1. Tulsi Dass and Satish K Sharma, Mathematical Methods in Classical and Quantum Physics, Universities Press 1998.
2. D. A. McQuarrie and John D Simon, Physical Chemistry, Viva Books, India 2003.
3. D. McQuarrie, Statistical Mechanics, University Science Books, 2000.

Reference Book
1. Chandler, D., Introduction to Modern Statistical Mechanics, Oxford University Press, 1987.
2. Biman Bagchi, Statistical Mechanics for Chemistry and Materials Science, CRC press, 2018.
4. Molecular Driving Forces: Statistical Thermodynamics in Chemistry and Biology by K. A. Dill and
1. S. Bromberg, Garland Science, 2003.

5. R Shankar, Basic Training in Mathematics, Springer, 2006.

Self-Learning Material

1. https://nptel.ac.in/courses/104101139
2. Course Introduction Basic Statistical Mechanics by Biman Bagchi
3. https://www.youtube.com/watch?v=M_dhvmM2fmI&list=PLOzRYVm0a65en9r kAeG_KDhh4thVEu5Od

Title	**Industrial Catalysis**	Course No.	CYL4XX0
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	B.S. in Engineering Chemistry and M.Sc. Chemistry	Type	Compulsory
Prerequisite			

Objectives

The Instructor will:

1. Impart knowledge on Catalysis and its importance.
2. Teach practical applications of catalysts applied in industry.

Learning Outcomes

1. The learners are expected to gain knowledge of independent thinking in designing, characterizing and fine tuning of catalysts suitable for potential catalytic transformations.
2. Learners will be able to translate fundamental catalytic knowledge to develop technology for industrial processes.
3. Learners will have an update on current trends and challenges of catalysis towards industrial application.

Contents

Introduction: Definition and concepts of catalysis, Activity, TOF, TON, selectivity, Homogeneous vs heterogeneous and biocatalysis **(4 Lectures)**
Homogeneous catalyzed Industrial processes: Hydrogenation, hydroformylation, carbonylation, wacker synthesis, oxo synthesis, C-C coupling reactions, Oligomerisation of ethylene (SHOP process), adiponitrile synthesis, polymerization, metathesis, Asymmetric catalysis, Monsanto L DOPA process, S-Naproxen, L-menthol **(14 Lectures)**
Industrial processes with Biocatalysts: Acrylamide, aspartame synthesis, pharmaceuticals, herbicides. **(4 Lectures)**
Heterogeneously catalyzed processes: Fischer Tropsch synthesis, water gas shift reaction, methanol synthesis, oxidation of propene. Refinery processes and petrochemistry. **(11 Lectures)**
Electrochemical reactions: Methanol oxidation, Catalytic processes with renewable materials, biofuels, biorefinery, phase transfer catalysis, catalysis reactor **(6 Lectures)**

Textbook

1. Hagen, J. Industrial Catalysis: A Practical Approach

Reference Books

1. Bhaduri S.; Mukesh, D. Homogeneous Catalysis: Mechanisms and Industrial Applications

Self-Learning Material

1. Industrial homogeneous Catalysis: Principles and Mechanisms by prof. debabrataMaiti, IIT Bombay, https://www.youtube.com/watch?v=GzXpURcjJwE&list=PL_uPpV3UHww2wyLk3XpR7LBqbR_2k1Fi0

Title	**Solid State and Materials Chemistry**	Course No.	CYL4XX0
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	B.S. in Engineering Chemistry and M.Sc. Chemistry	Type	Compulsory
Prerequisite			

Objectives

The Instructor will:

1. Provide an overview of the relationships between molecular or solid state structures and material properties.
2. Provide an interdisciplinary understanding of solid state chemistry which aims to provide an understanding of how molecular structure affects the properties of materials.

Learning Outcomes

The students are expected to have the ability to:

1. Obtain required knowledge for understanding material science problems and structure of solids.
2. Develop insight into electronic structure of crystals and compare it with the electronic structure of nanomaterials, chemical-physical fundamentals as well as basic method of characterisation of solids.

Contents

Structure of Solids: Crystalline and Amorphous, diffraction techniques, symmetry and point groups, packing in solids, classification, lattice energy, bonding, structures: NaCl, TiO_2, ZnS, wurtzite, Perovskite, covalent and ionic solids. (**10 Lectures**)
Crystal defects: non-stoichiometry, cluster, diffusion, Fick's Law and Kirkendall effect, Identification of defects using microscopic techniques. (**5 Lectures**)
Solid state reaction: Chemical and Physical Methods of preparation, reactivity of solids, decomposition mechanism, single crystal growth and thin film deposition. (**10 Lectures**)
Band theory: Intrinsic and extrinsic semiconductors, insulators, density of states, Dielectrics, Hall effect, Thomson, Peltier and Seeback effects. (**Lectures 8**)
Properties of Solids: Magnetic, Electrical and Optical properties, Different type of Magnetism and Superconductivity, Introduction to nanomaterials and properties. (**Lectures 6**)

Textbooks

1. West, A.R., (2015), *Solid State Chemistry and Its Applications*, 2nd edition, John Wiley & Sons
2. Lesley E Smart and Elaine E Moore, (2005), *Solid State Chemistry: An Introduction*, 3rd Edition, Taylor and Francis

Reference Books

1. Cheetham, A.K. and Day, P., (1997), *Solid State Chemistry Compounds*, 2nd Edition, Clarendon Press, Oxford
2. Harry R. Allcock, (2008), *Introduction to Materials Chemistry*, 1st Edition, Wiley.
3. C N R Rao and J Gopalkrishnan, (2004) *New Directions in Solid State Chemistry*, 2nd Edition, Cambridge.

Self Learning Material

Subramaniam, A, *Structure of Materials*, NPTEL Course Material, Department of Materials Science and Engineering, Indian Institute of Technology Kanpur, http://nptel.ac.in/courses/113104014/16

Elective Courses

Title	**Supramolecular Chemistry and Applications**	Course No.	CYL6XX0
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	B.S. in Engineering Chemistry and M.Sc. in Chemistry	Type	Elective
Prerequisite			

Objectives

The course aims to:

1. Develop a strong foundation in supramolecular chemistry.
2. Explain how non-covalent forces govern self-assembly and molecular recognition.

Learning Outcomes

By the end of the course, students will be able to:

1. Explain the role of non-covalent and host–guest interactions in supramolecular systems.
2. Apply supramolecular principles to advanced material design and their applications.

Contents

Fundamentals of Supramolecular Chemistry: Introduction and its historical development, non-covalent interactions, molecular recognition and complementarity, lock–key and induced fit models, positive and negative cooperativity, (**10 Lectures**)
Host–Guest Chemistry: Explores the synthesis, structure, and function of major host molecules (e.g., crown ethers, cryptands, calixarenes, cyclodextrins). Covers the governing principles of host-guest chemistry—pre-organisation, complementarity, and the lock-and-key model—in the binding of cationic, anionic, and neutral guests. (**9 Lectures**)
Self-Assembly in Supramolecular Architectures: Dynamic covalent chemistry, hierarchical self-assembly; supramolecular polymers and dynamic assemblies; molecular capsules and cages; rotaxanes and catenanes; molecular knots and mechanically interlocked molecules, stimuli-responsive systems. (**10 Lectures**)
Supramolecular Materials and Applications: Molecular machines, porous supramolecular materials; Metal–Organic Frameworks (MOFs) and covalent organic frameworks (COFs); basic principles of framework construction and topology and their applications. (**10 Lectures**)

Textbooks

1. Supramolecular Chemistry: Concepts and Perspectives, J.-M. Lehn, VCH, Weinheim, 1995.
3. Supramolecular Chemistry, J. W. Steed and J. L. Atwood, John Wiley & Sons, Chichester, 2009.

Reference Books

1. Applications of Supramolecular Chemistry, Edited By Hans-Jorg Schneider, CRC Press, 2012.

Online Resources

1. Chopra, D., Supramolecular Chemistry, NPTEL Course material, Department of Chemistry, IISER Bhopal https://nptel.ac.in/courses/104106683.
2. Bharadwaj, P. K., Supramolecular Chemistry, NPTEL course material, Department of Chemistry, Indian Institute of Technology, Kanpur, https://nptel.ac.in/courses/104104364

Title	**Polymer Material Science**	Course No.	CYL4XX0
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	B.S. in Engineering Chemistry	Type	Elective
Prerequisite			

Objectives

The instructor will:

1. Introduce the fundamental principles of polymer chemistry and materials science.
2. Provide comprehensive knowledge of modern polymer characterization techniques.
3. Enable students to critically interpret experimental data obtained from advanced analytical tools used in polymer science.

Learning Outcomes

The students are expected to:

1. Describe different polymer structures, architectures, and molecular weight distributions.
2. Explain the relationship between polymer structure, morphology, and thermal, mechanical, and physical properties.
3. Understand the principles and applications of key polymer characterization techniques.
4. Analyze and interpret polymer characterization data reported in scientific literature.

Contents

Introduction and Classification of Polymers: Definition and historical development of polymers, Polymer nomenclature and terminology, Classification of polymers (Homopolymers and copolymers, Thermoplastics and thermosets, Elastomers and vitrimer systems), Overview of polymer materials and their industrial importance **(8 Lectures)**.

Polymer Synthesis: Step-growth (condensation) polymerization, Chain-growth polymerization, Free radical polymerization, Controlled/living radical polymerization, Ionic polymerization (cationic and anionic), Ziegler-Natta polymerization, Coordination polymerization, Ring-opening polymerization, Strategies for designing functional polymers **(12 Lectures)**.

Introduction to Polymer Characterization Techniques: Molecular Weight Determination (Number average and weight average molecular weight, Light scattering techniques, Gel permeation chromatography (GPC), Spectroscopic Techniques (NMR, FTIR), Thermal Analysis (DSC, TGA), Microscopy Techniques (SEM, TEM, AFM) **(9 Lectures)**.

Polymer Processing and Industrial Applications: Extrusion, Injection molding, Compression molding, Automotive and aerospace materials, Electronic and electrical polymers, Biomedical polymers, Industrial coatings, adhesives, and elastomers **(5 Lectures)**.

Sustainability in Polymer Science: Biodegradable and bio-based polymers, Polymer recycling and sustainable materials development **(5 Lectures)**.

Textbook

1. P. C. Painter and M. M. Coleman: Fundamentals of Polymer Science, 2. ed., together with the problem sets.
2. Brydson's Plastics Materials, (1993), *Eighth edition*, J. A. Brydson's, edited by M Gilbert.

Reference Books

1. Polymer Chemistry by Charles E. Carraher, sixth edition.
2. The Chemistry of Polymers by John W. Nicholson, 3rd edition, RSC publishing.

Self Learning Material

1. Prof. Dibakar Dhara, IIT Kharagpur https://nptel.ac.in/courses/104105039/

Title	**Green Chemistry and Applications**	Course No.	CYL4XX0
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	B.S. in Engineering Chemistry	Type	Elective
Prerequisite			

Objectives

The course aims to:

1. Introduce fundamental principles, metrics, and concepts of green chemistry
2. Develop an understanding of green synthetic methods, catalytic strategies, and alternative reaction media for environmentally benign chemical processes.
3. Familiarize students with renewable resources, sustainable materials, and real-world applications of green chemistry in industry and society.

Learning Outcomes

By the end of the course, students will be able to:

1. Apply green chemistry metrics to quantify the sustainability of chemical reactions
2. Design environmentally benign synthetic routes using modern green methodologies.
3. Evaluate chemical technologies based on environmental, economic, and societal sustainability criteria.

Contents

Introduction to Green Chemistry: Definition and historical evolution of green chemistry, Environmental impact of traditional chemical processes, Global challenges and Indian context, Role of chemistry in sustainable development (**3 lectures**)

Principles and Metrics of Green Chemistry: The 12 principles of Green Chemistry, Atom Economy (AE), Environmental Factor (E-factor), Reaction Mass Efficiency (RME), Process Mass Intensity (PMI), Limitations of green chemistry metrics, Life Cycle Assessment (LCA) (**7 lectures**)

Green Synthetic Methods: Green solvent alternatives, green reagents, Solvent-free conditions, Microwave-assisted synthesis, Ultrasound-assisted synthesis, Mechanochemistry, Topochemical Synthesis, Catalysis in Green Chemistry, enzymatic transformation, (**10 lectures**)

Design of Green Processes and Sustainable Materials: Case studies in industrial green process design, Biomass as a chemical feedstock, Biofuels and biorefineries, Design of sustainable polymers, green routes to polymeric materials (**10 lectures**)

Applications: Green chemistry in the pharmaceutical industry, Agriculture, Dyes and Energy, Circular economy (**9 lectures**)

Text books

1. Green Chemistry: An Introductory Text, Mike Lancaster, Royal Society of Chemistry, 2010.
2. Green Chemistry and Catalysis, Roger A. Sheldon, Isabel Arends, Ulf Hanefeld, Wiley-VCH, 2007.
3. Renewable Resources for Green Chemistry, James H. Clark, Fabien E. I. Deswarte (Eds.), Royal Society of Chemistry, 2015.

Reference Books

1. Green Chemistry: An Inclusive Approach, Bela Török, Timothy Dransfield (Eds.), Elsevier, 2018.
2. Handbook of Green Chemistry, Volume 1: Green Catalysis - Homogeneous Catalysis, Paul T. Anastas, Robert H. Crabtree (Eds.), Wiley-VCH, 2009.
3. Handbook of Green Chemistry, Volume 2: Green Catalysis - Heterogeneous Catalysis, Paul T. Anastas, Robert H. Crabtree (Eds.), Wiley-VCH, 2009.

Title	**Organometallic Compounds in Organic Synthesis**	Course No.	CYL6XX0
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	B.S. in Engineering Chemistry	Type	Elective
Pre-requisite			

Objective

1. To introduce the fundamentals of organometallic compounds in Organic Synthesis with an emphasis on the modern methods.
2. Philosophy of organic synthesis, understanding of the organometallic reagents, and its role in organic synthesis and reaction mechanism.
3. Metal catalyzed method development and cascade approaches that helps in shaping academic as well as industrial research.

Learning Outcomes

The students are expected to have the ability to:

1. Understand the basic properties of organometallic compounds and their reactivity's
2. Differentiate between metals by their reactivity's and role in organic synthesis
3. Ability to design and develop the novel method/reactions utilizing organometallic catalysis

Contents

Brief history of metals: B, Li, Mg, Cu, Sn, Fe, Ru, Co, Zn and Ni, biological importance, nomenclature, 18e- rule, classification, preparation and properties, general reaction – transmetallation, oxidative addition reductive elimination and migratory insertion **(6 Lectures)**

B: Hydroboration-oxidation, Rearrangements, Allylboration, as reducing agent, Suzuki reaction and related reactions. **(4 Lectures)**

Li, Cu and Mg: Grignard and Organolithium Reagents, Gillman reagent, Conjugate addition, Ullmann reaction and Applications of BuLi and MeLi in the Reactions **(5 Lectures)**
Sn: Synthesis and reactions of organotin compounds, tributyltin azide, organostannane addition, tributyltin hydride in radical reactions, Stille reaction and reduction of organic compound **(5 Lectures)**
Ru: Regioselective Reductions, Oxidations, C-C bonds formation, Ruthenacycle Intermediates, Olefin Metathesis, Ring closing metathesis and Cyclopropanation **(5 Lectures)**
Fe: Polymerizations, oxidative couplings, oxidations, reductions, C- C bond formation, Ferrier rearrangement, one-pot multicomponent condensations, Friedel-Crafts reactions, Prins-type cyclisation, deprotection of various functional groups. **(5 Lectures)**
Co: Hydrogenation, hydro-functionalization, cycloaddition, radical and biomimetic reactions, cross-coupling, synthesis of heterocyclic compounds (Pauson-Khand) **(5 Lectures)**
Zn: Reductions of unsaturated compounds, oxidation, hydroamination, depolymerizations, transformations of carbon dioxide, oxidative coupling reactions, C-C, C-N, and C-O bond formation, Reformatsky reaction, Simmons–Smith reaction, Barbier reaction **(4 Lectures)**
Ni: Alkene/alkyne oligomerizations, Coupling reactions and Ni carbonylation. **(3 Lectures)**

Text Books

1. Shun-Ichi Murahashi: Ruthenium in Organic Synthesis, Wiley, 2004
2. Clayden, J., Greeves, N., and Warren, S., (2012), Organic Chemistry, 2nd Edition, Oxford

Reference Books

1. L. Brandsma, S.F. Vasilevsky and H.D. Verkruijsse: Application of Transition Metal Catalysts in Organic Synthesis, 9th edition, Springer, 1999
2. Jiro Tsuji: Transition Metal Reagents and Catalysts: Innovations in Organic Synthesis, 1st Edition, Wiley, 2002

Self-Learning Material
https://nptel.ac.in/content/storage2/courses/104103022/download/module11.pdf

Title	**C–H Bond Activation and Functionalization**	Course No.	CYL4XX0
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	B.S. in Engineering Chemistry	Type	Elective
Pre-requisite			

Objective
The instructor will guide to:

1. Develop a strong understanding of C–H activation strategies and mechanisms.
2. Apply C–H functionalisation in the synthesis of natural products and bioactive molecules.
3. Explore applications in medicinal chemistry, functional materials development, and industries.

Learning Outcomes
Students will be able to:

1. Explain the fundamental principles and mechanisms of C–H activation.

2. Apply C–H activation and functionalisation strategies to the synthesis of organic molecules.
3. Evaluate the applications of C–H activation in medicinal chemistry and materials science.

Contents

Fundamentals: Nature of C–H bonds; concept of C–H activation and functionalisation; key components involved in bond activation, thermodynamic and kinetic aspects, fundamental mechanisms including oxidative addition (OA), σ-bond metathesis (SBM), electrophilic substitution (ES), and concerted metalation–deprotonation (CMD). **(5 Lectures)**

Chelation-assisted C–H activation: strong vs weak chelation, monodentate and bidentate directing groups, removable and transient directing groups, strategies for remote C–H activation (meta- and para-selectivity), β- and γ-selectivity, template-assisted activation. **(5 Lectures)**

Nature and role of transition metals in C–H activation: comparison of noble metals (Pd, Rh, Ru, Ir) and base metals (Mn, Fe, Co, Cu, Ni) in catalysis. **(5 Lectures)**

Name reactions and types of C–H bond transformation: Murai reaction, Catellani reaction, Hartwig–Miyaura borylation, Fagnou arylation, Fujiwara–Moritani reaction, White–Chen oxidation, Trost indole alkylation, formation of C–C and C–X (X = B, P, O, N, F, S) bonds, cross-coupling and cascade reactions. **(10 Lectures)**

Green and Metal-free C-H bond functionalisations: Directed ortho-lithiation, Friedel–Crafts alkylation, Minisci and Hofmann–Löffler–Freytag (HLF) reactions, iodine-mediated transformations, photochemical, electrochemical, and organocatalytic approaches. **(4 Lectures)**

Photochemical and electrochemical C-H bond functionalization: Basics of photochemistry, Single Electron Transfer (SET), Energy Transfer (EnT), Hydrogen atom transfer (HAT) processes, Basics of electrochemistry, Anodic and cathodic activation pathways, Direct and mediated electrochemical oxidation, comparative analysis between photochemical vs electrochemical methods. **(6 Lectures)**

Applications of C-H functionalisation: cross-dehydrogenative couplings, total synthesis of natural products, late-stage functionalisation of bioactive molecules, synthesis of medicinal relevance, and efficient access to functional materials. **(4 Lectures)**

Text Books:

1. Yu, J.-Q., & Shi, Z. (Eds.). (2010). *C–H activation*. Springer.
2. Lersch, M., & Tilset, M. (Eds.). (2010). *Alkane C–H activation by single-site metal catalysis*. Springer.
3. Ackermann, L. (Ed.). (2015). *C–H and C–X bond functionalization: Transition metal mediation*. Royal Society of Chemistry.

Reference Books

1. Dixneuf, P. H., & Doucet, H. (Eds.). (2016). *C–H bond activation and catalytic functionalization* I and II. Springer.
2. Maiti, D. (Ed.). (2022). *Handbook of C–H functionalization*. Wiley-VCH.

Self-learning Material:

1. NPTEL, Prof. A. G. Samuelson, IISc Bangalore.
https://www.youtube.com/watch?v=C6G7X8WayEA

Title	**Chemistry of Organic Biomolecules**	Course No.	CYL6XX0
Department	Chemistry	L-T-P [C]	3-0-0 [3]
Offered for	M.Sc. Chemistry and B.S. in Engineering Chemistry	Type	Elective
Prerequisite			

Objectives

The instructor will:

1. Introduce students to structures and functions of organic biomolecules.
2. Impart comprehensive knowledge on chemical synthesis can be applied to engineer new biomolecules for modern applications.

Learning Outcomes

The students are expected to have the ability to:

1. Describe the structures, chemical properties, and functions of biomolecules.
2. Integrate fundamental concepts to conceptualize and design chemical technology for bio-applications.

Course Contents

Introduction: Organic chemistry of living systems, pH and buffers, Covalent and non-covalent interactions in organic and biological world, Analogy between organic chemistry and biochemical reactions (**3 Lectures**)

Chemistry of Amino Acids: Structure and properties of amino acids, amide-coupling reactions, amine/acid protection and deprotection protocols, Ninhydrin test for amino acids, Synthesis of non-canonical and unnatural amino acids and applications, Peptides and solid-state peptide synthesis, Protein secondary structure, Characterization of peptides and proteins using NMR, mass, etc. (**8 lectures**)

Chemistry of Enzymes: Classification and properties of enzymes, thermodynamics and kinetics of enzyme catalysis, catalytic mechanisms, enzyme inhibition and drug design, Industrial application of a few enzymes: in organic transformation and fermentation; enzyme as medicine/drug; Abzymes in organic transformation such as Diels Alder, Baldwin's rule, Oxy-Cope rearrangement (**6 lectures**)

Chemistry of Nucleic Acids: Sugars and organic bases; Nomenclature, Conformation of sugar-phosphate backbone, Nucleotide chemistry and tautomerism, Hydrogen bonding by bases, π-stacking interactions and DNA intercalators, Chemical synthesis and application of unnatural nucleosides in modern technologies (**7 lectures**)

Chemistry of carbohydrates and fatty acids: Carbohydrates: stereochemistry, Haworth and chair notations, epimers and anomers, mutarotation, glycosidic bonds, chemical synthesis and degradation of monosaccharides, nitrogen containing sugars, applications in drug delivery systems. Structure and types of lipids, chemical synthesis of artificial lipids for modern applications. (**10 lectures**)

Chemistry of terpenes, terpenoids and steroids: Classification, chemical structures, systematic nomenclature, Isoprene rule, Biosynthesis of terpenes and cyclization mechanisms and origin of non-classical carbocation rearrangement, cholesterol and its role; Biosynthesis; application of terpenes, such as Eucalyptus oil, Isolation techniques for industrial applications (**5 lectures**)

Textbooks

1. T. W. Graham Solomons, C. B. Fryhle, S. A. Snyder. Organic Chemistry. 12th Edition, Wiley.

2. D. V. Vranken and G. A. Weiss. *Introduction to Bioorganic Chemistry and Chemical Biology*. Garland Science; 1st edition, 2012
3. H. Dugas. *Bioorganic Chemistry: A Chemical Approach to Enzyme Action*. Springer-Verlag New York Inc.; 3rd Edition, 1996

Reference Books

1. The organic chemistry of enzyme-catalyzed reactions, by Richard B. Silverman, Academic Press, San Diego, 2000, 717 pp
2. J. E. McMurry. *The Organic Chemistry of Biological Pathways*. W.H.Freeman & Co Ltd; 2nd edition, 2015

Online Learning Material

1. S. S. Bag, Bio-organic chemistry, NPTEL Course Material, Department of Chemistry, Indian Institute of Technology Guwahati, https://archive.nptel.ac.in/courses/104/103/104103018/

Title	**Nanomaterials and Nanodevices**	Course No.	CYL6XX0
Department	Chemistry	L-T-P [C]	3-0-0 [3]
Offered for	B.S. in Engineering Chemistry	Type	Elective
Prerequisite			

Objectives

The Instructor will:

1. Underlying scientific basis for the behaviour of nanomaterials
2. Discuss methods of synthesis, fabrication and characterization of nanomaterials
3. Provide scope of nanomaterials and potential translation as products

Learning Outcomes

The students are expected to have the ability to:

1. Describe the basic science behind the properties of materials at the nanometer scale
2. Learn principles behind advanced experimental techniques for studying nanomaterials
3. Systematically solve scientific problems related specifically to Nano technological materials

Contents

Concepts, Definitions and Examples: Nanoscale processes, nanosystems, nanostructures, important nanomaterials such as clusters, nanocrystals, nanotubes and nanowires and 2D materials. (**2 Lectures**)

Size-dependent properties: Quantum confinement, quantum dots, Bandgap, Surface Ligands, Surface effects in nanosystems. Exciton dynamics, plasmonic properties, defect chemistry and surface states. Optical, mechanical, electronic and magnetic properties along with surface reactivity. (**10 Lectures**)

Synthesis of nanomaterials: Top-down and bottom-up, soft versus hard methods, chemical and physical methods, hybrid methods for synthesis of nanomaterials. (**6 Lectures**)

Experimental methods for the study of nanomaterials: Electron microscopes (SEM and TEM), scanning probe microscope (AFM and STM), X- ray diffraction (XRD), X- ray photoelectron spectroscopy (XPS), BET surface area, DLS, Zeta potential, electroanalytical techniques and miscellaneous methods. (**10 Lectures**)

Fabrication of Nanodevices: Concepts and methods; fabrication of nanodevices, solar cell, biosensors, photo detectors, photoelectrochemical, and electrochemical devices. (**5 Lectures)**

Applications: Applications for nanomaterials in biology, energy and environmental remediation. toxicity and environmental impact, and safe handling of nanomaterials. Translating nanomaterials and nanodevices into commercial products. (**6 lectures**)

Text Books

1. Pradeep, T., (2012), *Textbook of Nanoscience and Nanotechnology*, Mc Graw Hill
2. C. N. R. Rao, P. J. Thomas and G. U. Kulkarni (2007)Nanocrystals: Synthesis, Properties and Applications,Springer.

Reference Books

1. Nalwa, H. S., (2004), *Encyclopedia of Nanoscience and Nanotechnology*, Edition American Scientific Publishers, Los Angeles
2. Rao, C.N.R. and Govindaraj, A., (2005), *Nanotubes and nanowires*, RSC Publishing
3. C. N. R. Rao, P. J. Thomas and G. U. Kulkarni (2007)Nanocrystals: Synthesis, Properties and Applications,Springer.

Self Learning Material

1. Subramaniam, A., Balani, K. *Nanostructures and Nanomaterials: Characterization and Properties*, NPTEL Course Material, Department of Materials Science & Engineering, Indian Institute of Technology, Kanpur, http://nptel.ac.in/courses/118104008/:

Title	**Chemistry of the f-block elements**	Course No.	CYL6XX0
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	B.S. in Engineering Chemistry	Type	Elective
Prerequisite			

Objectives

The instructor will:

1. Provide sound knowledge of the lanthanides and actinides chemistry and related important compounds, and their application in practical purposes.

Learning Outcomes

The students are expected to have the ability to:

1. Understand fundamental aspects of lanthanide, actinide, and critical elements.
2. Appreciate reasons for their positioning in the periodic table
3. Apply the critical importance of these rare earth elements in the real world.

Contents

Introduction: Discovery and Positioning of Lanthanides and Actinides in periodic table and importance in modern technology. Difference from d block/main group elements **(5 Lectures)**

Rare Earth Elements: Coordination chemistry and periodic trends, electronic structure and magnetism, luminescence properties. Modern applications of rare earth elements chemistry including lanthanide ions as spectroscopic probes, sensors, NMR Shift reagents,

MRI contrast agents and strong magnets. Lanthanides in biology: Ln binding proteins **(15 Lectures)**
Separation Chemistry: Mining, Separation and Extraction Techniques for rare earth elements. **(2 Lectures)**
Chemistry of Actinide: Introduction, structure, bonding and reactivity of actinides and transactinides and application in radiopharmaceuticals (**8 Lectures)**
Organometallic compounds of f -block elements: Synthesis, structure, bonding and properties of metallocene, alkyl, aryl and cyclooctatetraene based complexes (**4 Lectures**)
f- block elements for small molecules activations and catalysis: Activation of Nitrogen, Hydrogen, Carbon dioxide and Carbon monoxide etc. Application in (Photo)catalysis and material chemistry. **(5 Lectures)**

Textbook
1. Lanthanide and Actinide Chemistry, Simon Cotton, John Wiley & Sons, Ltd. 2006
2. Luminescence of Lanthanide Ions in Coordination Compounds and Nanomaterials, Ed. Ana de Bettencourt–Dias , John Wiley and Sons, Ltd, 2014
3. Lanthanides and Actinides in Molecular Magnetism, Ed. R. A. Layfield, M. Murugesu, Wiley-VCH, 2015

Reference Books
1. The Lanthanides And Actinides: Synthesis, Reactivity, Properties And Applications (World Scientific)
2. Organometallic and coordination chemistry of the actinides D.M.P. Mingos Volume Editor T.E. Albrecht- Schmitt (Springer)
4. d- and f- block Chemistry – Chris Jones (RSC)
5. The f-elements – Nikolas Kaltsoyannis and Peter Scott (OUP)

Self-Learning Material
1. Lecture by Prof. Joseph Cotruvo of Penn State University USA
   https://www.youtube.com/watch?v=uRvVuDv5d4I

Title	**Ligand Design: Principles and Applications**	Course No.	CYL4XX0
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	B.S. in Engineering Chemistry	Type	Elective
Prerequisite			

Objectives
The instructor will:
1. Appreciate the basic principles of ligand design for transition metal chemistry and their application in catalysis.
2. Introduce different classes of ligands and their applications.

Learning Outcomes
By the end of this lesson, the student will be able to:
1. Identify the role of ligands in controlling the structure, stability, and reactivity of metal complexes.

2. Evaluate steric effects in promoting selectivity and preventing catalyst deactivation.
3. Predict how ligand tuning alters reaction pathways and kinetics.

Contents

Fundamentals: Classification of ligands: Anionic, neutral and Z-type of ligands; Electronic effects; steric effects and cone angle concept; HSAB principle and ligand preference **(4 lectures)**

Electronic Structure and Reactivity: Metal-ligand bonding models (Crystal field theory, Ligand field theory, Molecular orbital approach); Oxidation state and electron counting method; Influence of ligand effects on reaction mechanism **(8 lectures)**

Ligand Classes and Architectures: Phosphine ligands; N-heterocyclic carbene ligands; Pincer and chelating ligands; redox-active and non-innocent ligands; directing ligands; supramolecular and multifunctional ligand systems **(8 lectures)**

Ligand Design for Catalysis: Cross-coupling reactions (ligand effect on Pd- and Ni-catalyzed coupling reaction); Buchwald coupling- ligand changes with the generation catalyst and their effect on substrate selectivity; Ligand-controlled hydrogenation and hydrofunctionalizations **(7 lectures)**

Asymmetric Catalysis: principles of chiral ligand design; Binap, Box, Salen and related ligand families; correlation between ligand structures and catalytic outcome **(5 lectures)**

Emerging concepts in ligand design: Metal ligand Cooperativity (MLC), FLP in metal catalysis, Green Chemistry and sustainable ligand design. Ligand effects in photoredox and electrocatalysis. **(7 Lectures)**

Textbooks

1. Ligand Design in Metal Chemistry, M. Stradiotto, R. Lundgren. (2016) Wiley.
2. Chiral Ligands, M. Dieguez. 2021 Routledge Publication

Reference Book

1. The Organometallic Chemistry of the Transition Metals – Robert H. Crabtree, Wiley (2014).
2. Organotransition Metal Chemistry: From Bonding to Catalysis – John F. Hartwig, University Science Books (2010).

Self-Learning Material

1. https://www.youtube.com/watch?v=Od94BSJ1JIw
2. Prof. A. G. Samuelson, IISC Bangalore https://nptel.ac.in/courses/104108062

Title	**Advanced Main Group Chemistry**	Course No.	CYL6XX0
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	B.S. in Engineering Chemistry	Type	Elective
Prerequisite			

Objectives

The instructor will:

1. Give insights into the interesting class of main group organometallics and other compounds.

2. Impart knowledge on recent advances in reactivity and catalytic applications of the main group compounds relevant to industrial applications.
3. Examine the roles of p-block compounds in materials science, agriculture, energy, and electronics, highlighting the connection between structure–property relationships and modern applications.

Learning Outcomes

The students are expected to:

1. Appreciate the interesting class of main group organometallic compounds.
2. Be updated on recent trends in the reactivity and catalytic applications of novel main-group compounds and their mechanistic understanding for further explorations.

Contents

Introduction: Structure, and bonding consideration of main group compounds (**5 Lectures**)

Synthesis, structure, and reactivity: Organo-alkali, alkaline earth metal-based compounds; Group 11 and 12 compounds. (**10 Lectures**)

Representative Chemistry of Group 13, 14, 15, and 16: Organoboron compounds, boron-based reduction, hydroboration, carboboration; (organo)aluminium compounds, hydroalumination, carboalumination, use of aluminium alkyls in polymerization of olefins; Chemistry of CO, and CO_2, persistent carbenes, organosilanes, organogermanes, organotin compounds. N_2 activation and reactions, nitrogen fixation, processes for NH_3 synthesis, oxides of nitrogen (N_2O, NO), and their reactivity study. Synthesis, structure, and reactivity of phosphorus and Bismuth compounds; sulfur and selenium-based compounds. Frustrated Lewis pairs (FLP). (**12 Lectures**)

Modes of activation in catalysis: Lewis acid/base, Bronsted acid/base, redox-active, Metallomimetics. **(3 lectures)**

Applications: GaAs, GaN, and $InSnO_3$: synthesis and applications in solar cells, activation, synthetic and catalytic applications of main group organometallic compounds, FLP Catalysis (**9 Lectures**)

Textbook

1. C. Elschenbroich (2006), Organometallics, 3rd edition, Wiley
2. A. J. Elias (2019), The Chemistry of the p-Block Elements, Universities Press
3. D. Shriver and P. Atkins, Inorganic Chemistry: Fifth Edition, Oxford.
4. F. A. Cotton, G. Wilkinson, C. A. Murillo, and M. Bochmann, Advanced Inorganic Chemistry: Sixth Edition, John Wiley Interscience

References Book

1. M. Bochmann (2014), Organometallics and Catalysis: An introduction, Oxford University press

Self-learning Material:

1. Balakrishna, M. S., *Chemistry of Main Group Elements*, NPTEL Course Material, Department of Chemistry, Indian Institute of Technology Bombay, http://nptel.ac.in/courses/117101105/
2. **https://nptel.ac.in/courses/104101090**

Title	**Electrode Materials**	Course No.	CYL4XX0
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	B.S. in Engineering Chemistry	Type	Elective
Prerequisite			

Objectives

The instructor will:

1. To transmit knowledge on understanding and designing electrodes in electrochemical cells towards sustainable green energy.

Learning outcomes:

1. The learners are expected to gain knowledge on electrochemical cells and electrodes as well as design principles and materials-specific issues of electrochemical cells for potential sustainable green energy.
2. Learners will have an update on current trends and challenges in designing electrode materials for efficient energy storage and conversion towards sustainable green energy.

Contents

Introduction: Fundamentals concept of electrodes (working, reference, and counter), roles of supporting electrolytes in electrochemistry, electrode–electrolyte interface, two electrodes vs. three electrodes measurements, classification of cells and batteries, galvanic cell, electrolytic cell and fuel cell, electrochemical rate constant, Nernst equation. **(8 Lectures)**

Electrocatalysis: Electrocatalytic hydrogen and oxygen evolution reaction, overpotential, Tafel plot, exchange current density, Faradaic efficiency, kinetics. **(3 Lectures)**

Electrode materials in electrocatalysis: Basics of electrode fabrication, conventional electrode materials including metal and alloys, metal oxide, carbon-based electrodes, Amorphous electrode and composite electrode materials, conductive polymer, semiconducting crystalline nanomaterials. **(6 Lectures)**

Energy storage and rechargeable alkali-ion battery: Lithium-ion (Li-ion) batteries, principle of operation, commercial Li-ion battery, anode materials in Li-ion battery: Li metal, intercalative materials, transition metal oxides, polyanionic compound, fluoride-based compounds. Synthesis and characterization techniques of Li-ion battery electrode materials. Beyond Li-ion: electrode materials for sodium-and magnesium-ion batteries. **(8 Lectures)**

Supercapacitor in storage technologies: Supercapacitors, difference between batteries and capacitors, working principal and storage mechanism of supercapacitor, galvanostatic charging/discharging, role of electrode materials in charge storage in capacitor, commonly used electrode materials in super capacitor. **(3 Lectures)**

Modern energy storage technologies: Commercial cathode and anode materials and battery chemistries in zinc-manganese battery, nickel-cadmium battery, nickel hydrogen battery, lead-acid battery, metal-air and metal-sulphur batteries. **(6 Lectures)**

Advanced batteries for electric vehicles: General characteristics and performance requirements for advanced rechargeable batteries, near-term rechargeable batteries for electric vehicles, fast-charging electrode design, refuellable batteries, thermal stability and safety. **(5 Lectures)**

Textbook

1. Electrochemical Methods: Fundamentals and Applications, 2nd Edition; Allen J. Bard, Larry R. Faulkner

2. Handbook of Battery Materials Editor(s): Dr.-Ing. Claus Daniel, Jürgen O. Besenhard
3. Electrode Materials for Energy Storage and Conversion by Mesfin A. Kebede and Fabian I. Ezema

Reference Books

1. Lithium-Ion Battery Chemistries by John T. Warner
2. Electrochemical Water Electrolysis Fundamentals and Technologies by Lei Zhang, Hongbin Zhao, David P. Wilkinson, Xueliang Sun, Jiujun Zhang

Self-Learning Material

1. YouTube channels such as NPTEL, MIT lectures, and university-level electrochemistry content. MIT Open Course Ware.

Course Title	**Water Chemistry**	Course No.	CYL4XX0
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	B.S. in Engineering Chemistry	Type	Elective
Pre-requisite			

Objectives

The instructor will:

1. A fundamental and advance understanding of the chemical and biochemical processes that are involved in water treatment for drinking purposes and treatment of industrial and domestic wastewaters for water reuse and discharge to the environment.
2. Provide knowledge of the key chemical processes relevant to research in water chemistry

Learning Outcomes

The students are expected to:

1. Perform quantitative and qualitative interpretations for water quality analysis
2. Apply concepts of chemical equilibrium to solve water related practical problems

Course Contents

Polar nature of water, Acids and bases, Buffering capacity of water (**3 Lectures**)
Equilibrium constant expressions, aqueous system including concentration, activities, activity coefficients and pH of equilibrium. (**4 Lectures**)
Chemical reaction equation and Arrhenius and Bronsted-Lowry acids and bases (**4 Lectures**)
Ionization constant reactions and expressions, Self-Ionization of water, Solubility-product expressions (**4 Lectures**)
Measuring pH, Filtration of various solids, Alkalinity and aqueous titrations (**3 Lectures**)
Cycling of water and residence time (**3 Lectures**)
Water availability,usage, quality and water treatment methods (**5 Lectures**)
Analytical methods for water quality analysis, and Statistical analysis of analytical data (**6 lectures**)

Reference Books

1. Sawyer, C., McCarty, P., & Parkin G, *Chemistry for Environmental and Engineering Science*. 5th Edition. Toronto: McGraw-Hill, 2003
2. Mark M. Benjamin, 2015, Water Chemistry, Waveland Press, Second Edition, ISBN 1-4786- 2308-X

Text Books

1. Werner Stumm, James J. Morgan, *Aquatic Chemistry: Chemical Equilibria and Rates in Natural Waters, 3rd Edition*, Wiley
2. Kerry J. Howe, David W. Hand, John C. Crittenden, R. Rhodes Trussell, *Principles of Water Treatment*, George Tchobanoglous, Wiley

Self Learning Material

1. NPTEL Lectures: https://nptel.ac.in/courses/122106030/

Title	**Chemical Binding**	Course No.	CYL6XX0
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	B.S. in Engineering Chemistry and M.Sc. Chemistry	Type	Elective
Prerequisite			

Objectives

The Instructor will:

1. Provide high level understanding of a chemical bond using quantum mechanics.
2. Describe knowledge of modern techniques in quantum chemistry

Learning Outcomes

The students are expected to have the ability to:

1. Use modern quantum chemistry techniques to solve fundamental problems related to basic chemistry
2. Understand a chemical bond

Contents

Electronic structure: Variation theory, perturbation theory, electron spin, He atom, Pauli exclusion principle, Slater determinant (**10 Lectures**)
Electronic structure of diatomic molecules: Born Oppenheimer approximation, Atomic units, H_2^+ ion, H_2 molecule, VB theory, MO theory, Semi-empirical methods (**10 Lectures**)
Wave function based theory: Hartree-Fock theory, Electron correlation, Self-consistent field wave function, Moller-Plesset theory, Coupled cluster formulation (**15 Lectures**)
Density functional theory (DFT): Principles of density functional theory, commercial functionals and applications (**4 Lectures**)

Textbook

1. Levine, I. N., *Quantum Chemistry*, Pearson education (2000).
2. Lowe, J. P., *Elementary Quantum Chemistry*, Academic Press.

Reference Books

1. Szabo, A. and Ostlund, N. S., *Modern Quantum Chemistry*, Dover (1996).

Title	**Principles of Fluorescence Spectroscopy and Imaging**	Course No.	CYL6XX0
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	B.S. in Engineering Chemistry	Type	Elective
Pre-requisite			

Objectives

1. The course is intended for individuals wishing an in-depth introduction to the principles of fluorescence spectroscopy and it's applications to the materials and life sciences.
2. It will also give in-depth knowledge of fluorescence imaging technology and how it can be useful for advanced research.

Learning Outcomes

1. Students will understand the importance of fluorescence imaging as a tool to solve a diverse range of problems in chemistry and biology.
2. They will have an understanding to determine dynamics in nano to femto-second time scale.
3. Students will have an understanding of cutting-edge single molecule imaging technology.

Contents

Introduction to Fluorescence Spectroscopy: Jablonski diagram, Stokes shift, Fluorescence lifetimes and quantum yields, Steady-state vs time-resolved fluorescence spectroscopy, Fluorophores (dyes, quantum dots and fluorescent proteins) and instrumentation, Quenching of Fluorescence: Stern-Volmer equation, Static and dynamic quenching, Application of quenching to protein, membrane and molecular biology, Mechanisms and dynamics of quenching. (**13 Lectures**)

Time-correlated single photon counting (TCSPC): Fluorescence lifetime or decay time, theory, principle, instrumentation and application of TCSPC, Solvent and temperature effect of lifetime, Dynamics of solvent and spectral relaxation, Time-domain life-time measurement, Fluorescence Anisotropy, femtosecond up-conversion spectroscopy, solvation dynamics, proton transfer (**13 Lectures**)

Single molecule spectroscopy: Principle of Single Molecule Fluorescence Resonance Energy Transfer (smFRET), Theory of FRET, Time dependent FRET, Application of FRET to understand conformational distributions and dynamics. Multiphoton Excitation and Microscopy, Fluorescence lifetime imaging (FILM), Single molecule imaging of protein and DNA, Fluorescence correlation spectroscopy (FCS), Application of FCS and single-molecule FRET, Applications of 2-photon excitation time-resolved confocal microscope (**13 Lectures**)

Text Book

1. Lakowicz, J. R. (2006) *Principles of Fluorescence Spectroscopy*, 3rd Edition, Springer

2. Murphy, D.B., and Devidson, M. W., (2001), *Fundamentals of Light Microscopy and Electronic Imaging*, 2nd Edition, Wiley-Blackwell

Reference Books

1. Valeur, B. (2001) *Molecular Fluorescence: Principles and Applications*, 2nd Ed. Wiley-VCH
2. Smith, A.;Gell, C. and Brockwell, D. (2006) *Handbook of Single Molecule Fluorescence Spectroscopy*, Oxford University Press

Self-Learning Material

1. Sen, P., *Basics of Fluorescence Spectroscopy*, NPTEL Course Material, Department of Chemistry, Indian Institute of Technology Kanpur https://nptel.ac.in/courses/104104084/
2. Dutta, A. *Ultrafast Laser Spectroscopy*, NPTEL Course Material, Department of Chemistry, Indian Institute of Technology Bombay https://nptel.ac.in/courses/104/101/104101122/

Title	**Single Molecule Spectroscopy**	Course No.	CYL4XX0
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	B.S. in Engineering Chemistry	Type	Elective
Prerequisite			

Objectives

The Instructor will:

This course will discuss advanced level theory, instrumentation and application of various single-molecule imaging techniques

Learning Outcomes:

The students are expected to:

Students will learn theory, instrumentation and lab experiments for single-molecule imaging

Contents

Introduction: History of single-molecule spectroscopy, Burst analysis, photon-counting histogram, smFRET and applications, measurements from immobilized samples, Molecular dynamics of single-molecules. Instrumentation and Microscopy **(14 Lectures)**

Correlation Spectroscopy: Correlation vs cross-correlation, Theory of FCS, molecular dynamics by FCS, quantum dot and single-molecule behavior, Applications of FCS **(9 Lectures)**

Applications: Confirmation Dynamics, Dynamic mechanism of biomolecule, Force and multi-parameter spectroscopy, Nanoscale-microscopy and high resolution imaging in individual cells. single-molecule enzyme Kinetics, nanopores. Application of various single-molecule imaging - tracking, ion-flux, protein-protein and protein-ligand interactions. **(11 Lectures)**

Lab experiments: smFRET experiment of DNA Holliday Junction using prism-type TIRF Microscope **(4 Lectures)**

Textbook

1. Grasland, Riglar and Widengren, Single-molecule Spectroscopy in chemistry, Physics and BIology, Nobel Symposium, Springer
2. Gell, Brockwell and Smith, Handbook on Single-molecule Fluorescence Spectroscopy, Oxford University Press
3. Elson and Rigler, Fluorescence correlation spectroscopy – Theory and Applications, Springer, (2012)

Reference Books

1. Lakowicz, J. R., (2006), Principles of Fluorescence Spectroscopy, 3rd Edition, Springer, New York

Self-Learning Material

1. iBiology, Biophysics, UCSF https://www.ibiology.org/research-talks/biophysics/

Title	**Theoretical account of Spectroscopy**	Course No	CYL4XX0
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	B.S. in Engineering Chemistry	Type	Elective
Prerequisite			

Objectives

The Instructor will:

1. Introduce to the basic principles of physical chemistry, quantum mechanics and classical electrodynamics to understand molecular spectroscopy.
2. Enable students to apply quantum mechanics to understand light-matter interaction as well as application of various spectroscopic techniques.

Learning Outcomes

The students are expected to have the ability to:

1. Understand the theoretical background of various spectroscopic techniques.
2. Connect quantum mechanical description of atomic and molecular structure and spectra of atoms and molecules over a wide range of wavelength.

Contents

Introduction and overview: Electromagnetic waves and polarization, Macroscopic view of light-matter interaction, Blackbody radiation, Einstein A and B coefficient, quantum description of matter, Time dependent perturbation theory, Fermi's Golden rule, hydrogen atoms, polyelectronic atoms, atomic term symbols, selection rules (**8 Lectures**)
Molecular Symmetry: Symmetry operations, point groups, character table, spectroscopic term symbols for describing atomic and molecular states, total representation of a group, symmetry and dipole moment (**4 Lectures**)
Rotational Spectroscopy: Classical description of molecular rotation, the rigid rotor, Rotational levels and transition rules, Rotational energy levels of diatomic molecules, energy levels of spherical and symmetric tops, moment of inertia, calculations of bond lengths and bond angles of simple triatomic molecules, vibrational stretching and

vibrational satellites, no-rigid rotor, centrifugal distortion, degeneracies and intensities, Stark effect, selection rules, rotational spectra of polyatomic molecules (9 **Lectures**)
Vibrational spectroscopy: classical description of molecular vibrations, the classical harmonic oscillator, quantum mechanics of molecular vibration, vibrational selection rules, anharmonic vibrations and Morse oscillator, bond dissociation energies and Birge-Sponer plots, calculation of force constants from vibrational spectrum, isotopic shift, rotational structure in vibrational spectra of diatomic molecules, vibration of polyatomic molecules, normal modes, Rotation-vibration spectra of diatomic molecules and calculation of molecular parameters (9 **Lectures**)
Electronic Spectroscopy: Basic principle, Born-Oppenheimer approximation, energy of electronic transition, selection rules, the Franck-Condon principle, Electronic transitions of polyatomic molecules, Molecular orbitals, Rovibronic transitions, vibrational coarse structure, Russel-Saunders spin-orbit coupling, absorption intensity, probability of light absorption, electronic spectra, classification of electronic transition, d-d and CT transitions (9 **Lectures**)

Textbook

1. Bernath, P. F., (2005), *Spectra of Atoms and Molecules*, 2nd Edition, Oxford University Press
2. Hollas, J.M (2013), Modern Spectroscopy, Wiley

Reference Books

1. Bunker, P.R., and Jensen, P. 2012. Molecular Symmetry and Spectroscopy. E-book edition. NRC Research Press, Ottawa, Ontario, Canada. 748 p
2. Hollas, J. M. 2013, High Resolution Spectroscopy, Elsevier Science

Self-Learning Material

1. Mangal Sundar, K., *Introduction to Quantum Chemistry and Molecular Spectroscopy,* NPTEL Course Material, Department of Chemistry, Indian Institute of Technology Madras, http:// http://nptel.ac.in/courses/104106083
2. Dutta, A., *Molecular Spectroscopy: A Physical Chemist's perspective*, NPTEL Course Material, Department of Chemistry, Indian Institute of Technology Bombay, http:// https://nptel.ac.in/courses/104101099

Course Title	**Principles of Biological Soft Matter**	Course No.	CY6XX0
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	B.S. in Engineering Chemistry and M.Sc. in Chemistry	Type	Elective
Pre-requisite			

Objectives

The instructor will:

1. To understand basic principles and theory of biological soft matter
2. To understand structure-property relationship of biological soft matter

Learning Outcomes
The students are expected to:

1. Integrate concepts from biology, chemistry, physics, and mathematics to understand biophysics
2. connect structure, simulation, and functions of protein, membrane

Contents

Fundamentals of Soft Matter: time, length and energy scales of soft matter; intermolecular forces; macromolecules; colloids, liquid crystals, amphiphilc self-assembly (**10 Lectures**)
Soft matter in Nature: Nucleic acids; structure, folding, interactions of proteins; polysaccharide, Different lipids and membrane structure, functions, Membrane Enzymes, Receptor, Transporter, channel, water, Active matter in living system (**15 Lectures**)
Statistical Mechanics and soft matter: Entropy, 2^{nd} law of thermodynamics, energy, temperature, free energy, distribution functions; random walk, fluctuations, simulations, introduction to the theory of active matter (**14 Lectures**)

Textbooks

1. Jones, R. A. L., Soft Condensed Matter, Oxford University Press 2002.
2. Jacob N. Israelachvili, Intermolecular and Surface Forces, Academic Press, 2011.
3. Anders Liljas, Lars Liljas, Miriam-Rose Ash, Goeran Lindblom, Poul Nissen, Morten Kjeldgaard,
4. Textbook of Structural Biology, World Scientific, 2020.

Reference Books

1. Mary Luckey, Membrane Structural Biology, Cambridge University Press, 2013.
2. Alexander Yu. Grosberg and Alexei R. Khokhlov, Statistical Physics of Macromolecules, AIP Press, 1994
3. M. P. Allen and D. J. Tildesley, Computer Simulation of Liquids, Clarendon Press, 1991.

Self-Learning Material

1. NPTEL course by Profs. Sunil Kumar, P. B., and Menon, G. I.,; "Physics of Soft Condensed Matter"; https://nptel.ac.in/syllabus/115106063/
2. Membrane BioPhysics and Membrane Proteins, https://www.youtube.com/watch?v=Fict6w40dJ0

Title	**Machine Learning for Chemistry**	Number	CYL6XX0
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	BS in Engineering Chemistry	Type	Elective
Prerequisite			

Objectives

The Instructor will:

1. Fundamental concepts and mathematical understanding of ML architecture will be detailed starting from a very basic background to students in basic sciences. Visual illustrations and animations will be used to make it more prominent to them.
2. Fundamental resemblance of manual scientific tools and primary machine learning algorithms will be highlighted such that students find it easy to transfer their ideas from science to the problem solving ability of machine-learning.
3. The course will start from a very basic background of solving problems of science and will be fetched toward solving the same problems and rather complex ones with a much compact and automated ML models with the usage of TensorFlow, keras and scikit learn.

Learning Outcomes

4. They will be able to recognize the problem specific nature of ML models and which problem will need which kind of ML model.
5. Students will be confident enough to build simple ML models themselves to solve their own scientific problems.
6. Mixing fundamental mathematical concepts with hands-on example programming assignment problems, this course has been designed to make students efficient to create ML architecture from scratch.

Contents

Supervised Learning Approach: Impact of AI in modern science, Recap of linear algebra, applications of machine learning in scientific problems of fitting data to models, idea of machine learning and regression, linear regression with examples from scientific data, Regression with multiple variables, feature engineering, polynomial regression, logistic regression, decision boundary, Problem of overfitting data, cost function and regularization, bias, variance, cross validation, Application in Classification of molecules in terms of toxicity, molecular structure and biological activity, molecular fingerprints, quantification of molecular properties for a new molecule from known Structure-property data. **(15 Lectures)**

Unsupervised Learning: Clustering, K-means algorithm, optimization objective, normal distribution, anomaly detection, Principle component analysis, Problems namely clustering of structural, dynamical and spectroscopic data, protein sequence identification aligning bio-activity and binding affinity to targets to be shown by unsupervised learning **(6 Lectures)**

Advanced Learning Algorithms in Case Studies: Neurons and brains, example of digit recognition, image processing, neural network layers, inference, forward and backpropagation, data in TensorFlow, efficient implementation of neural-networks in TensorFlow, binary and multiclass classification, activation functions, one hot encoders, continuous valued features, autoencoders and deep graph neural networks in crystal structure prediction and material properties, sampling with replacement, random forest algorithm, usage of neural networks in PES curve fitting and catalyst design, decision tree, searching efficient reaction pathway and neural networks in rare-event simulations, applications in protein sequence-mediated structure prediction with RFdiffusion/alphafold/ProteinMPNN, prediction of melting temperature for biomolecules and ionic liquids, designing effective collective variables in free-energy estimation, efficient automated coarse-grained forcefield design, high-throughput biomolecule-ligand binding efficiency estimation and finding active binding sites **(18 Lectures)**

Textbooks

1. Alpaydim, E.; An Introduction to Machine Learning (**(Adaptive Computation and Machine Learning series),** The MIT Press (24 March 2020), **ISBN-13:** 978-0262043793
2. Andrew N.G.; Machine Learning Yearning, GitHub; eBook (Draft, 2018); eBook (MIT Licensed), **ISBN-13:** 978-1999579500
3. Kelleher, J.D., Namee, B. M. and D'Arcy, A.; Fundamentals of Machine Learning for Predictive Data Analytics: Algorithms, Worked Examples, and Case Studies; The MIT Press; 2nd edition (20 October 2020), **ISBN-13 :** 978-0262044691

Reference books

1. Pattern Recognition and Machine Learning, Christopher M. Bishop, Springer, ISBN-13 : 978-1493938438
2. Mohri, M., Rostamizadeh, A., Talwalkar, A., Bach, F.; Foundations of Machine Learning, MIT Press (7 September 2012), ISBN-13 : 978-0262018258
3. Courville, A., Goodfellow, I. and Bengio, Y.; Deep Learning (Adaptive Computation and Machine Learning Series), MIT Press (18 November 2016); The MIT Press, ISBN-13 : 978-0262035613
4. Theobald, O.; Machine Learning for Absolute Beginners: Python for Data Science; Scatterplot Press (1 January 2021); **ISBN-13 :** 978-1913666521

Self-Learning Materials

1. Andrew N. G., Geoff Ladwig, Aarti Bagul, Eddy Shyu, Stanford Machine Learning Specialization, https://www.coursera.org/specializations/machine-learning-introduction

2. Stanford CS229: Machine Learning by Andrew NG, https://www.youtube.com/watch?v=vStJoetOxJg