Malaviya National Institute of Technology Jaipur

Course Structure and Syllabus for B.Tech. (Minor in Chemistry)

Department of Chemistry

Proposed Course Structure of B. Tech. (Minor in Chemical Sciences)

Course Details (Credits: 18)

S. No.	Course Code	Title of the course	Subject Area	L-T-P	Credits
1.	24CYTXXX	New Energy Materials	PC	3-0-0	3
2.	24CYTXXX	Sustainable Chemical Syntheses	PC	3-0-0	3
3.	24CYTXXX	Modern Instrumental Methods in Chemical Analyses	PC	3-0-0	3
4.	24CYPXXX	Advanced Chemistry Lab	PC	0-0-6	3
5.	24CYTXXX	Program Elective I	PE	3-0-0	3
6.	24CYTXXX	Program Elective II	PE	3-0-0	3
		Total			18

List of Program Electives (I and II) offered by the Department of Chemistry

S.No	Course Code	Program Electives	L-T-P	Credits
1	24CYTXXX	Photo-Inorganic Chemistry	3-0-0	3
2	24CYTXXX	Supramolecular Chemistry	3-0-0	3
3	24CYTXXX	Polymer Chemistry	3-0-0	3
4	24CYTXXX	Organometallic Chemistry of Main Group Elements	3-0-0	3
5	24CYTXXX	Bio-Inorganic Chemistry	3-0-0	3
6	24CYTXXX	Symmetry and Group Theory	3-0-0	3
7	24CYTXXX	Organic Synthesis	3-0-0	3
8	24CYTXXX	Applied Biocatalysis (Enzymes)	3-0-0	3
9	24CYTXXX	Heterocyclic Chemistry	3-0-0	3
10	24CYTXXX	Cell Structure and Biomolecules	3-0-0	3
11	24CYTXXX	Bio Chemistry	3-0-0	3
12	24CYTXXX	Physical Organic Chemistry	3-0-0	3
13	24CYTXXX	Electrochemistry: Ionics and Electrodics	3-0-0	3
14	24CYTXXX	Advanced Analytical Chemistry	3-0-0	3

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15	24CYTXXX	Molecular Spectroscopy	3-0-0	3
16	24CYTXXX	Concepts in Chemical Kinetics and Dynamics	3-0-0	3
17	24CYTXXX	Environmental Chemistry	3-0-0	3
18	24CYTXXX	Introduction to Density Functional Theory	3-0-0	3
19	24CYTXXX	Atmospheric Chemistry	3-0-0	3
20	24CYTXXX	Introduction to Astrochemistry	3-0-0	3
22	24CYTXXX	Crystallography	3-0-0	3
23	24CYTXXX	Solid State Chemistry-Fundamentals and Applications	3-0-0	3
24	24CYTXXX	Laser Spectroscopy: Theory and Applications	3-0-0	3

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Department of Chemistry

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Proposed Course Structure of B. Tech. (Minor in Chemistry)

Course Details (Credits: 18)

S. No.	Course Code	Title of the course	Subject Area	L-T-P	Credits
1.	24CYTXXX	New Energy Materials	PC	3-0-0	3
2.	24CYTXXX	Sustainable Chemical Syntheses	PC	3-0-0	3
3.	24CYTXXX	Modern Instrumental Methods in Chemical Analyses	PC	3-0-0	3
4.	24CYPXXX	Advanced Chemistry Lab	PC	0-0-6	3
5.		Program Elective I	PE	3-0-0	3
6.		Program Elective II	PE	3-0-0	3
		Total			18

MALAVIYA NATIONAL INSTITUTE OF TECHNOLOGY JAIPUR

DEPARTMENT OF CHEMISTRY

DETAILS OF THE COURSE

Course Type	Course Code	Course Title	Credits	Lecture	Tutorial	Practical	Studio
PC	24CYTXXX	New Energy Materials	3	3	0	0	0

PREREQUISITE

Basic understanding of Physical and Inorganic Chemistry

COURSE OBJECTIVE(s)

1. To offer knowledge on various energy and power generation systems, highlighting the imperative role of materials and their functioning in these systems.
2. To realize how new materials can make improvement in energy harvesting, energy transformation and energy storage processes.

COURSE OUTCOMES:

CO1	Learn fundamentals of various energy technologies
CO2	Understand the concept of materials for energy application
CO3	Impart knowledge on analyzing energy materials' structure and properties

COURSE ASSESSMENT

The Course Assessment (culminating to the final grade) will be made up of the following three components:

S. No.	Component	Weightage
a)	Internal assessment (based upon assignments, quizzes and attendance)	20%
b)	Mid-term examination	30%
c)	End Semester Examination	50%

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COURSE CONTENTS

Unit I: Introduction to energy harvesting, transformation, and storage systems; thermal, chemical, and electrochemical processes in energy systems; efficiency evaluation of the energy conversion and storage systems; structures and property behaviors of energy materials; advanced characterization methods of energy materials.

(No. of lectures: 8)

Unit II: Materials for solar cells, hydrogen generation, water splitting, energy catalysis, piezoelectric energy harvesting systems, non-rechargeable batteries, ion-batteries, Zn/MnO_2 "alkaline" cells, Li/FeS_2 cells, Li/I_2 batteries, Zn/Air cells, Mg and Al based cells, sodium/sulfur batteries, flow batteries, ZEBRA batteries, high temperature batteries, low- and high-temperature fuel cells, supercapacitors, electrochemical flow capacitors, all-solid-state and wearable supercapacitors, supercapatteries; testing methodologies of various energy systems.

(No. of lectures: 16)

UNIT III: Nanostructurization of materials for energy systems; Nano-architectured current collectors and current collector/active film interface; nanofabrication techniques; vacuum/ electron beam evaporation methods, sputtering, chemical vapor/atomic layer/pulsed laser deposition, molecular beam epitaxy, lithography, and mechanical milling methods to prepare energy materials; chemical self-assembly, colloidal synthesis, hydrothermal synthesis, all-solid-state synthesis, and microwave synthesis methods of zero-, one, two and three-dimensional energy materials; future perspective of new energy materials. **(No. of lectures: 12)**

TEXT BOOKS/ REFERENCE BOOKS: -

1. Energy Materials: Fundamentals to applications by Sanjay J. Dhoble, N. Thejo Kalyani, B. Vengadaesvaran, Abdul Kariem Arof. Elsevier, 2021.
2. Energy Materials Discovery: Enabling a sustainable future by Geoffrey A. Ozin; Joel Y. Y. Loh. Royal Society of Chemistry, 2022.
3. Energy Materials by Duncan W. Bruce, Dermot O'Hare, Richard I. Walton. John Wiley & Sons, Ltd., 2011.
4. Introduction to Materials for Advanced Energy Systems by Colin Tong. Springer Cham. 2018.

Lecture Plan

Lecture No.	Topics to be covered
1	Introduction to energy harvesting systems
2	Common energy transformation systems
3	Fundamentals of energy storage systems
4	Thermal and chemical processes in energy systems
5	Electrochemical processes in energy systems
6	Efficiency evaluation of the energy conversion and storage systems
7	Structures and property behaviors of energy materials
8	Advanced characterization methods of energy materials
9	Materials for solar cells
10	Hydrogen generation systems
11	Materials for water splitting systems
12	Materials for energy catalysis
13	Piezoelectric energy harvesting systems
14	Non-rechargeable batteries
15	Ion-batteries
16	Zn/MnO_2 "alkaline" cells
17	Li/FeS_2 cells and Li/I_2 batteries
18	Zn/Air cells
19	Mg and Al based cells
20	Sodium/sulfur batteries
21	Flow batteries
22	ZEBRA batteries and high temperature batteries

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23	Low- and high-temperature fuel cell
24	Supercapacitors and electrochemical flow capacitors
25	All-solid-state and wearable supercapacitors, supercapatteries
26	Testing methodologies of various energy systems
27	Nanostructurization of materials for energy systems
28	Nano-architectured current collectors and current collector/active film interface
29	Nanofabrication techniques
30	Vacuum/electron beam evaporation methods to prepare materials
31	Sputtering, chemical vapor/atomic layer/pulsed laser deposition methods to prepare materials
32	Molecular beam epitaxy, lithography, and mechanical milling methods to prepare materials
33	Chemical self-assembly and colloidal synthesis methods to prepare materials
34	Hydrothermal synthesis to prepare materials
35	All-solid-state and microwave synthesis methods to prepare materials
36	Future perspective of new energy materials

DETAILS OF THE COURSE

Course Type	Course Code	Course Title	Credits	Lecture	Tutorial	Practical	Studio
PC	24CYTXXX	Sustainable Chemical Syntheses	3	3	0	0	0

PREREQUISITE

Basic knowledge of Stoichiometric and Catalytic Chemical Reactions

COURSE OBJECTIVE(s)

This course aims to provide future chemists and engineers with the tools required to minimize the environmental impact of chemicals and chemical processes. The course highlights and emphasizes designing environmentally friendly chemical processes (Green Chemistry) that are both economically and technologically feasible.

COURSE OUTCOMES:

CO1	To learn the fundamental philosophy and the latest developments in sustainable chemistry.
CO2	To understand why solvent replacements are being sought.
CO3	To familiarize with different green reaction alternatives of conventional reaction procedures with real world applications.
CO4	To understand how waste biomass can be converted to wealth.
CO5	To understand importance of recycling and its application in circular economy

COURSE ASSESSMENT

The Course Assessment (culminating to the final grade) will be made up of the following three components:

S. No.	Component	Weightage
d)	Internal assessment (based upon assignments, quizzes and attendance)	20%
e)	Mid-term examination	30%
f)	End Semester Examination	50%

COURSE CONTENTS

Module 1 (6L)	**Fundamental:** Basic Concepts of Sustainable Chemistry; Sustainability assessment; Essentials of sustainable chemistry; Role of chemistry in sustainability.
Module 2 (10L)	**Green Chemistry:** Principles of green chemistry; Designing safer chemicals, Predict the properties and environmental aspects before synthesis; Use of catalysts to reduce time and energy demands, Minimize waste; Design for energy efficiency, Least energy intensive route for synthesis. **Green Solvents:** Atom economy, Metathesis; Ionic liquids, Classification, Synthesis & applications; Deep eutectic solvents, classification, Synthesis & applications; Supercritical fluids, Preparation and various applications.
Module 3 (10L)	**Green Synthetic Methods:** Safer Chemical Design; Green chemistry, Molecular design pyramid, Safer chemical design examples. Green alternative of conventional synthetic methods; Green catalysis (Phase Transfer Catalysts, Chitosan, enzymes), Solvent free reactions, Microwave assisted reactions, Examples of green synthesis-Ibuprofen. Industrial Green Improvements of Consumer Products; Vitamin C Synthesis using enzymes (Hoffman La Roche), Zoloft -Presidential Chemistry, Award Winning Innovation (Pfizer), Methyl Methacrylate, syngas process (Eastman Chemicals).DOZN score for the synthesis of chemical compounds, Real world applications of green chemistry
Module 4 (10L)	**Value addition to Waste Biomass:** Renewable Feed stocks; Types of biomass derived fuels & energy, Biogas, Bioethanol, Biodiesel; Thermochemical conversion, Gasification pathway, Pyrolysis pathway; Biochemical conversion, Anaerobic digestion, Fermentation. Application of Renewable Raw Materials in organic synthesis: Historical developments-Alizarine, Indigo and Coniine synthesis. Application of Renewable Raw Materials in synthesis: Synthesis of (±)-Usnic acid from lignin, tetracyclin antibiotics from Chitin derived L-Rednose, (−)-Bissetone and (−)-palythazine from cellulose derived glucose. Biodegradable polymers (PEF, PLA, PBS and PHA) and their applications. Synthesis of biodegradable polymers.Plastic recycling in circular economy. Sustainable packaging. Life Cycle Analysis (LCA), Cradle to grave and Cradle to

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	Cradle design.

TEXT BOOKS/ REFERENCE BOOKS: -

1. New trends in Green chemistry: V. K. Ahluwalia, M. Kidwai Anamaya Publishers
2. Introduction to Green Chemistry: Albert S. Matlack, 2nd edition, CRC Press
3.Waste to Wealth-The circular economy advantage: Peter Lacy and JakobRutqvist, Ma Editions
4.Green Solvents-Ionic Liquids: Paul T. Anastas (Series Editor), Peter Wasserscheid, Annegret Stark, Wiley-VCH
5. Sustainable chemistry: G. Reniers and C.A Brebbia, WIT Press
6. Valorization of biomass to value added commodities: Daramola, Michael, Ayeni, and Augustine (Eds), Springer

Lecture Plan

Lecture No.	Topics to be covered
1	Basic Concepts of Sustainable Chemistry
2	Basic Concepts of Sustainable Chemistry
3	Sustainability assessment
4	Essentials of sustainable chemistry
5	Essentials of sustainable chemistry
6	Role of chemistry in sustainability
7	Principles of green chemistry
8	Principles of green chemistry
9	Designing safer chemicals, predict the properties and environmental aspects before synthesis
10	Designing safer chemicals, predict the properties and environmental aspects before synthesis
11	Use of catalysts to reduce time and energy demands, minimize waste
12	Design for energy efficiency, least energy intensive route for synthesis.
13	Atom economy, metathesis
14	Ionic liquids, classification, synthesis & applications
15	Deep eutectic solvents - classification, synthesis & applications
16	Supercritical fluids, preparation and various applications.

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17	Safer Chemical Design; Green Chemistry Molecular design pyramid
18	Safer Chemical Design; Green Chemistry Molecular design pyramid
19	Green alternative of conventional synthetic methods; Green catalysis (Phase Transfer Catalysts, Chitosan, enzymes)
20	Green alternative of conventional synthetic methods; Green catalysis (Phase Transfer Catalysts, Chitosan, enzymes)
21	solvent free reactions, Microwave assisted reactions
22	Examples of Green Synthesis-Ibuprofen. Industrial Green Improvements of Consumer Products
23	Examples of Green Synthesis-Ibuprofen. Industrial Green Improvements of Consumer Products
24	Vitamin C Synthesis using enzymes (Hoffman La Roche), Zoloft - Presidential Chemistry Award Winning Innovation (Pfizer)
25	Methyl Methacrylate syngas process (Eastman Chemicals), DOZN score for the synthesis of chemical compounds.
26	Real world applications of green chemistry
27	Types of biomass derived fuels & energy, biogas, bioethanol, biodiesel
28	Thermochemical conversion, gasification pathway, pyrolysis pathway
29	Thermochemical conversion, gasification pathway, pyrolysis pathway
30	Biochemical Conversion, anaerobic digestion, fermentation
31	Application of Renewable Raw Materials in organic synthesis
32	Historical developments- Alizarine, Indigo and Coniine synthesis
33	Synthesis of (±)-Usnic acid from lignin, tetracyclin antibiotics from Chitin derived L-Rednose, (−)-Bissetone and (−)-palythazine from cellulose derived glucose
34	Biodegradable polymers (PEF, PLA, PBS and PHA) and their applications
35	Synthesis of biodegradable polymers.Plastic recycling in circular economy. Sustainable packaging. Life Cycle Analysis (LCA), Cradle to grave and Cradle to Cradle design
36	Summarization on our learning

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DETAILS OF THE COURSE

Course Type	Course Code	Course Title	Credits	Lecture	Tutorial	Practical	Studio
PC	24CYTXXX	Modern Instrumental Methods in Chemical Analyses	3	3	0	0	0

PREREQUISITE
None

COURSE OBJECTIVE(s)
This course aims to gain a deep understanding of the fundamental principles of advanced methods of chemical analyses. Specifically, molecular spectroscopic techniques will be focussed. Emphasis will be given to problem solving, where student will gain understanding of the outcomes of each spectroscopic method in real life applications (Pharmaceuticals and renewable energy devices).

COURSE OUTCOMES:

CO1	Understand the basics of Spectroscopic methods of chemical analyses
CO2	Real life problem solving to analyse chemical structures using spectroscopy
CO3	Understand the application of electronic spectroscopy including device engineering with special emphasis on renewable energy devices
CO4	Understand the basic principles of nuclear magnetic resonance and real life problem solving of analysing molecules using NMR.
CO5	Understand the preparative methods of chromatographic sample purifications and understand the quantitative and qualitative applications of chromatographic techniques.
CO6	Understand the fundamentals of electrochemical characterization techniques and understand the redox behaviours of chemical systems.

COURSE ASSESSMENT
The Course Assessment (culminating to the final grade) will be made up of the following three components:

S. No.	Component	Weightage
1.	Internal assessment (based upon assignments, quizzes and attendance)	20%
2.	Mid-term examination	30%
3.	End Semester Examination	50%

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COURSE CONTENTS

1. **Basics Principles:**
   Electromagnetic radiation, Regions of Spectrum, Basic elements of practical spectroscopy, Signal to Noise: Resolving power, Width, and Intensity of Spectral transitions, Fourier Transformation Spectroscopy. Applications of Infrared spectroscopy in Chemical Analyses. (8 h).

2. **Basics and Applications of Electronic Spectroscopy in Molecules:**
   Molecular Absorption and Emission, Beer-Lambert Law, Kasha's Principle, Quantum Yields and Lifetime Measurements, Instrumentation, Molecular Engineering to control the absorption and emission properties, Energy transfer processes, Photosensitizers, Solar Cells, Hydrogen energy device engineering by tuning electronic structure. (12 h)

3. **Nuclear Magnetic Resonance Spectroscopy in Chemical Analyses:**
   Instrumentation and basic principles, Chemical Shift, Spin-Spin coupling, Peak intensity, Structure elucidation of organic molecules using NMR spectroscopy, Interpretation of NMR of simple molecules, Effect of hydrogen bonding, Applications of NMR **(8 h)**

4. **Chromatographic Methods:**
   Principles of Chromatographic separation, Concept of theoretical plates, Van-Deemter Equation, Column Chromatography, Gas Chromatography: Packed and capillary column, Stationary phases, FID, and TCD detectors, Quantitative and qualitative analyses of samples. **(6 h)**

5. **Basics Electrochemical Techniques:**
   Introduction, electrochemical cell; Reference Electrodes-Hydrogen gas electrode, Saturated calomel electrode, Silver/silver chloride; electrodes-electrodes; Basic Electrode Processes, Cyclic voltammetry, Interpretation of curves, reversibility parameters, Differential Pulsed voltammetry. **(4 h)**

TEXT BOOKS/ REFERENCE BOOKS: -

- Analytical Chemistry, 7th Edition, 2013, Gary D. Christian, Purnendu K. Dasgupta, Kevin A. Schug, ISBN: 978-0-470-88757-8.
- Spectrometric identification of organic compounds (Fifth Edition) R. M. Silverstein, G. C. Bassler And T. C. Morrill. Wiley, New York, 1991.
- Organic Spectroscopy: Principles and Applications, 2020, II edition. ISBN: 978-81-7319-566-2.
- A Practical Beginners guide to cyclic voltammetry, Jillian Dempsey, et al., *J. Chem. Educ.* 2018, 95, 2, 197-206. https://doi.org/10.1021/acs.jchemed.7b00361.

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Lecture Plan

Lecture No.	Topics to be covered
1	Electromagnetic radiation, Regions of Spectrum,
2	Basic elements of practical spectroscopy,
3	Signal to Noise ratio, Resolving power, Width, and Intensity of Spectral transitions
4	Fourier Transformation Spectroscopy and Instrumentation
5	Applications of Infrared spectroscopy in Chemical Analyses
6	Structure evaluation using IR spectra: Simple molecules
7	Structure evaluation using IR spectra: Simple molecules
8	Structure evaluation using IR spectra: Metal Carbonyl complexes and complex molecules
9	Molecular Absorption Beer-Lambert Law
10	Emission: Fluorescence and Phosphorescence including Kasha's Principle
11	Quantum Yields: Relative and Absolute measurements. Instrumentation
12	Lifetime Measurements (special reference to TCSPC)
13	Molecular Engineering to control the absorption and emission properties. Organic Reactions for ligand Syntheses.
14	Molecular Engineering to control the absorption and emission properties. Transition metal complexes wrt SOC concept.
15	Energy transfer processes
16	Photosensitizers: Inorganic and Organic dyes (including standard ligand groups)
17	Solar Cells: DSSCs and Efficiency Measurements
18	IPCE curves and Analyses of Performance
19	Hydrogen energy device engineering and Efficiency Measurements
20	TANDEM cells for Hydrogen production: Instrumentation and examples with quantification experiments
21	Instrumentation and basic principles of NMR
22	Chemical Shift, Spin-Spin coupling,
23	Peak intensity
24	Structure elucidation of organic molecules using NMR spectroscopy,
25	Interpretation of NMR of simple molecules, Effect of hydrogen bonding,
26	Interpretation of NMR of simple molecules
27	Interpretation of NMR of simple molecules
28	Interpretation of NMR of simple molecules
29	Principles of Chromatographic separation: 1
30	Principles of Chromatographic separation: 2
31	Concept of Theoretical plates and Van-Deemter Equation,

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32	Column Chromatography
33	Gas Chromatography: Packed and capillary column, Stationary phases, FID, and TCD detectors,
34	Quantitative and qualitative analyses of samples.
35	Introduction, electrochemical cell; Reference Electrodes-Hydrogen gas electrode, Saturated calomel electrode, Silver/silver chloride; electrodes-electrodes; Basic Electrode Processes,
36	Cyclic voltammetry, Interpretation of curves, reversibility parameters,
37	Differential Pulsed voltammetry
38	Analyses Electrochemical data of Inorganic complexes

DETAILS OF THE COURSE

Course Type	Course Code	Course Title	Credits	Lecture	Tutorial	Practical	Studio
PC	24CYTXXX	Advanced Chemistry Lab	3	0	0	6	0

PREREQUISITE

Basic understanding of fundamental Chemistry

COURSE OBJECTIVE(s)

1. To familiarize the students with the practice of experimental chemistry
2. Handling of sophisticated instruments

COURSE OUTCOMES:

CO1	Use different instrumental methods of analysis and estimation.
CO2	Design and conduct experiments.
CO3	Students will be able to understand importance of analytical tools in industry as well as in day-by-day applications.
CO4	Synthesize chemical compounds and gain hands on practice of handling laboratory equipment

COURSE ASSESSMENT

The Course Assessment (culminating to the final grade) will be made up of the following three components:

S. No.	Component	Weightage
1	Internal assessment (based upon	20%

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	assignments, quizzes and attendance)	
2	Mid-term examination	30%
3	End Semester Examination	50%

COURSE CONTENTS

6. **Basics Principles:**
Electromagnetic radiation, Regions of Spectrum, Basic elements of practical spectroscopy, Signal to Noise: Resolving power, Width, and Intensity of Spectral transitions, Fourier Transformation Spectroscopy. Applications of Infrared spectroscopy in Chemical Analyses. (8 h).

7. **Basics and Applications of Electronic Spectroscopy in Molecules:**
Molecular Absorption and Emission, Beer-Lambert Law, Kasha's Principle, Quantum Yields and Lifetime Measurements, Instrumentation, Molecular Engineering to control the absorption and emission properties, Energy transfer processes, Photosensitizers, Solar Cells, Hydrogen energy device engineering by tuning electronic structure. (12 h)

8. **Nuclear Magnetic Resonance Spectroscopy in Chemical Analyses:**
Instrumentation and basic principles, Chemical Shift, Spin-Spin coupling, Peak intensity, Structure elucidation of organic molecules using NMR spectroscopy, Interpretation of NMR of simple molecules, Effect of hydrogen bonding, Applications of NMR **(8 h)**

9. **Chromatographic Methods:**
Principles of Chromatographic separation, Concept of theoretical plates, Van-Deemter Equation, Column Chromatography, Gas Chromatography: Packed and capillary column, Stationary phases, FID, and TCD detectors, Quantitative and qualitative analyses of samples. **(6 h)**

10. **Basics Electrochemical Techniques:**
Introduction, electrochemical cell; Reference Electrodes-Hydrogen gas electrode, Saturated calomel electrode, Silver/silver chloride; electrodes-electrodes; Basic Electrode Processes, Cyclic voltammetry, Interpretation of curves, reversibility parameters, Differential Pulsed voltammetry. **(4 h)**

TEXT BOOKS/ REFERENCE BOOKS: -

1. Mendham J., Denny R.C., Barnes J.D. and Thomas M.J.K., "Vogel's Text Book of Quantitative Chemical Analysis" 6th Ed., Pearson Education 2004.
2. Ewing G.W., "Instrumental Methods of Chemical Analysis", 5th Ed., McGraw Hill. 2004
3. A Collection of Interesting General Chemistry Experiments, A.J. Elias, Universities Press, 2002.
4. Experiments and Techniques in Organic Chemistry, D.P. Pasto, C. Johnson and M. Miller, Prentice Hall.
5. C.Garland, J. Nibler and D.Shoemaker, Experiments in Physical Chemistry, McGrawHill Education; 8th Edn., 2008

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6. B. Viswanathan and P. S. Raghavan, Practical Physical Chemistry, Viva Books Pvt. Ltd.

Lecture Plan

Lecture No.	Topics to be covered
Experiment 1	Determination of organochlorine pesticides in food by gas chromatography.
Experiment 2	Determination of ascorbic acid in vitamin-C tablet or lemon.
Experiment 3	Estimation of copper in brass.
Experiment 4	Column chromatographic separation of organic/inorganic mixtures.
Experiment 5	Determination of COD of given water sample.
Experiment 6	Preparation and characterization of Boric Acid.
Experiment 7	Color effect due to ligand exchange in Ni/ Co/ Fe complexes.
Experiment 8	To determine the number of chloride ions in the $[Co(NH_3)_5]Cl_3$ and $[Co(NH_3)_5Cl]Cl_2$
Experiment 9	$10Dq=\Delta_o$ measurements of hexaaqua complexes of 1st series transition metals.
Experiment 10	Acetylation of salicylic acid (Aspirin), aniline, and other organic molecules.
Experiment 11	Estimating amines/phenols using bromate bromide solution/or acetylation method.
Experiment 12	Determination of Saponification values of an oil sample.
Experiment 13	Isolation, extraction, and separation (crystallization) of caffeine from tea leaves.
Experiment 14	Isolation and Extraction of casein from milk.
Experiment 15	Conductometric determination of critical micellar concentration.
Experiment 16	Determination of the molecular formula of copper-ammonia complex by the partition coefficient method
Experiment 17	Determination of specific rotation of tartaric acid by polarimetric method.
Experiment 18	Determination of metal-ligand complex composition by job's method.

DETAILS OF THE COURSE

Course Type	Course Code	Course Title	Credits	Lecture	Tutorial	Practical	Studio
PC	24CYTXX	Photo-Inorganic	3	3	0	0	0

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	X	Chemistry					

PREREQUISITE

None

COURSE OBJECTIVE(s)

This course aims to gain a deep understanding of the fundamental principles of photochemistry. Student will understand how the photochemical systems function. Device fabrication aspects with respect to solar cells and other renewable energy devices and cancer therapy will be introduced.

Course Outcomes

CO1. Understand the underlining physical principles that govern the light emitting devises.
CO2. Understand the role of inorganic and organometallic complexes in the step towards clean energy devices.
CO3. To familiarize with techniques and methods that have direct implication in developing new materials.

COURSE ASSESSMENT

The Course Assessment (culminating to the final grade) will be made up of the following three components;

S. No.	Component	Weightage
g)	Internal assessment (based upon assignments, quizzes and attendance)	20%
h)	Mid-term examination	30%
i)	End Semester Examination	50%

COURSE CONTENTS

Module 1 (12L) **Introduction to Molecular Photophysics and Photochemistry**
Molecular Absorption and Emission Spectra, Instrumentation, Basic laws of Photochemistry, Beer Lambert law, Jablonski diagram, Calculation of fluorescence rate constants from absorption spectra-Dipole and transition moments, selection rules-Rate constants of internal conversion; the energy gap law-Rate constants of inter system crossing, Sayed rules-Kasha and Vavilov rules-Franck-Condon Principle-Energy transfer, Excimer, Exciplex, quenching and sensitization.

Module 2 (8 L) **Techniques and Methods for Engineering Perspective**
Light sources, filters, monochromator, and detectors-Preparative Irradiation-Absorption Spectra-Steady state emission spectra-Time resolved luminescence-Quantum yields: Differential quantum yield-Actinometry-Spectrophotometric determination of the reaction progress-Luminescence quantum yields-Stern-Volmer analysis-Quantum yields of triplet formation-Experimental arrangements for quantum yield measurements.

Module 3 (16 L) **Applications**
Transition Metal Complexes as photosensitizers, Dye-Sensitized solar

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cells, Perovskites solar cells, Factors affecting the efficiency, Device Fabrication, Incident to Photon Conversion efficiency (IPCE), Sunlight to chemical feedstocks, Photo-electrochemical cells, fabrication aspects, efficiency studies, Photochemical Hydrogen generation, Drawbacks of using 1st row transition metals in P-V devices, resolving efficiency issues through ligand design, Transition metal complexes in flexible displays, device structure of OLEDs, thermally activated delayed fluorescence, color tuning, aggregation induced emission, organometallic complexes in sensing applications, Photodynamic therapy.

TEXT BOOKS/ REFERENCE BOOKS: -

1. Principles of Fluorescence Spectroscopy, Lakowicz, III-Edition, Springer.
2. Highly Efficient OLEDs with Phosphorescent Materials, Hartmut Yersin, 2007, Wiley-VCH.
3. Organic Photochemistry and Photophysics, V. Ramamurthy, Kirk S. Schanze, CRC Press.
4. Photochemistry and Photophysics: Concepts, Research, Applications, Vincenzo Balzani, Paola Ceroni, Alberto Juris, 2014.

Lecture Plan

Lecture No.	Topics to be covered
1-3	Molecular Absorption and Emission Spectra, Instrumentation, Basic laws of Photochemistry, Beer Lambert law, Jablonski diagram.
4-5	Calculation of fluorescence rate constants from absorption spectra
6-7	selection rules-Rate constants of internal conversion; the energy gap law-Rate constants of inter system crossing
8	Sayed rules-Kasha and Vavilov rules
9-10	Franck-Condon principle-Energy transfer
11-12	Excimer, Exciplex, quenching and sensitization
13	Light Sources
14	Filters and Monochromators and detectors
15	Irradiation-Absorption Spectra-Steady state emission spectra
16	Time resolved luminescence-Quantum yields: Differential quantum yield
17-18	Actinometry-Spectrophotometric determination of the reaction progress
19-20	Luminescence quantum yields-Stern-Volmer analysis-Quantum yields of triplet formation-Experimental arrangements for quantum yield measurements
21-22	Transition Metal Complexes as photosensitizers
23	Dye-Sensitized solar cells
24	Perovskites solar cells
25	Factors affecting the efficiency and Device Fabrication
26	Incident to Photon Conversion efficiency (IPCE)
27	Sunlight to chemical feedstocks
28	Photo-electrochemical cells, fabrication aspects, efficiency studies, Photochemical Hydrogen generation
29	Drawbacks of using 1st row transition metals in P-V devices, resolving efficiency issues through ligand design

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30	Transition metal complexes in flexible displays, device structure of OLEDs,
31-32	Thermally activated delayed fluorescence, color tuning, aggregation induced emission
33-34	Organometallic complexes in sensing applications
35-36	Photodynamic Therapy

DETAILS OF THE COURSE

Course Type	Course Code	Course Title	Credits	Lecture	Tutorial	Practical	Studio
PC	(24CYTxx x)	Supramolecular Chemistry	3	3	0	0	0

PREREQUISITE

Basic knowledge of different chemical bonds

COURSE OBJECTIVE(s)

To impart knowledge of types of supramolecular Chemistry, structures-bonding and their applications as Organic materials, sensors, and devices

COURSE OUTCOMES:

CO 1	The students will acquire knowledge of molecular recognition and nature of bindings involved in biological systems
CO 2	The students will acquire knowledge of structures of various supramolecular structure in solution and solid state
CO 3	The students will acquire knowledge on applications of supramolecular compounds in miniaturization of molecular devices-Molecular machine and switches

COURSE ASSESSMENT

The Course Assessment (culminating to the final grade) will be made up of the following three components;

S. No.	Component	Weightage
a)	Internal assessment (based upon assignments, quizzes and attendance)	20%
b)	Mid-term examination	30%
c)	End Semester Examination	50%

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COURSE CONTENTS

Unit 1 (8 L)	**Introduction:** Basic concept and principles; Molecular recognition, Nature of interactions in supramolecular structures: Definition, Structure and Stability, strength, Secondary Electrostatic Interactions in Hydrogen Bonding Arrays and Non-covalent interactions. Supramolecular chemistry in life.
Unit 2 (8 L)	**Host–guest Chemistry**: Structures of crown ethers, Cryptands, Cyclodextrins, Cryptophanes, Host-guest interactions, Preorganization and complementarity, Lock and key analogy, binding of cationic, Anionic, Ion pair and neutral guest molecules.
Unit 3 (6 L)	**Self-assemblies in Supramolecular Chemistry**: Self-assembled molecules: Catenanes, Rotaxanes, Dendrimers and Supramolecular gels. Biomimicking chemistry. Metal organic frameworks.
Unit 4 (14 L)	**Molecular Devices**: Molecular Electronic devices, Molecular wires, Molecular rectifiers, Molecular Switches and Molecular logic gates. Examples of recent developments in supramolecular chemistry from current literature.

TEXT BOOKS/ REFERENCE BOOKS: -

1. Lehn, J. M., Supramolecular Chemistry-Concepts and Perspectives, Wiley –VCH (1995).
2. Beer, P.D., Gale, P. A., and Smith, D. K., Supramolecular Chemistry, Oxford University Press (1999).
3. Steed, J. W., and Atwood, J. L., Supramolecular Chemistry, Wiley (2000).
4. Crystal Engineering. The Design of Organic Solids by G.R. Desiraju, Elsevier, 1989.

Lecture Plan

Lecture No.	Topics to be covered
1	Discussion on concept and development of supramolecular chemistry - history
2	Discussion on ion-ion, ion-dipole, dipole-dipole interactions
3	Discussion on H-bonding interactions in supramolecular chemistry
4	Discussion on cation-π and anion-π interactions
5	Discussion on π-π interactions in supramolecular chemistry
6	Discussion on van der Waal interactions in supramolecular chemistry
7	Comparison among different supramolecular energies with respect to their energy and possibilities

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8	Porphyrin and other tetra-pyrrole macrocycles
9	Supramolecular chemistry in Life
10	Summarization on our learning
11	Discussion on crown ethers
12	Discussion on Cryptands
13	Cyclodextrins and its uses
14	Cyclodextrins and its uses
15	Discussion on Host-guest interactions, preorganization and complementarity
16	Discussion on Host-guest interactions, Preorganization and complementarity
17	Lock and key analogy, binding of cationic and Anionic guest molecule
18	Interactions with ion pair and neutral guest molecules
19	Discussion on key recent developments
20	Summarization on our learning
21	Design and synthesis of self-assembled molecules – new properties
22	Continued discussion on design and synthesis of self-assembled molecules – new properties
23	Discussion on self-assembly by H-bonding
24	Catenanes and Rotaxanes – design and synthesis
25	Catenanes and Rotaxanes – uses and future potential applications
26	Synthesis of artificial helixes – classification – potential applications
27	Synthesis of artificial helixes – classification – potential applications
28	Development by Prof. J-M, Lehn Noble laureate in supramolecular chemistry
29	Supramolecular gels – design and synthesis – potential uses
30	Supramolecular gels – design and synthesis – potential uses
31	Relevance of supramolecular chemistry to mimic biological system.
32	Summarization on our learning
33	Molecular electronic devices, molecular wires, molecular rectifiers
34	Molecular switches and molecular logic gates
35	Discussion on key recent developments
36	Discussion on key recent developments

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DETAILS OF THE COURSE

Course Type	Course Code	Course Title	Credits	Lecture	Tutorial	Practical	Studio
PE	(24CYTXXX)	Polymer Chemistry	3	3	0	0	0

PREREQUISITE

Basic knowledge of Chemistry

COURSE OBJECTIVE(s)

1. To impart the knowledge of basic concepts of the polymers.
2. To provide the knowledge of polymer chemistry based on synthesis, characterization and applications.

COURSE OUTCOMES:

CO 1	Students will be able to explain the classification of various types of polymers.
CO 2	Student will understand the different methods for the synthesis and characterization of the polymers.
CO 3	Students will be able to demonstrate the ability to quickly acquire the knowledge of new polymer-related applications and development of new polymer materials and related processes with respect to sustainability considerations

COURSE ASSESSMENT

The Course Assessment (culminating to the final grade) will be made up of the following three components;

S. No.	Component	Weightage
1.	Internal assessment (based upon assignments, quizzes and attendance)	20%
2.	Mid-term examination	30%
3.	End-term Examination	50%

COURSE CONTENTS

Module 1 (10L)	**Introduction** Introductory concepts, definition, monomers, repeat units, degree of polymerization, linear, branched and network polymers, characterization: molecular weight studies and molecular weight distribution, determination of thermal parameters, importance of polymers, Mechanistic aspects: addition, ionic, emulsion, suspension, aqueous, coordination, condensation polymerization.
Module 2 (10L)	**Classification and Polymerization** Classification of polymers, polymerization in homogeneous and heterogeneous systems, step-growth syntheses, chain polymerizations, ring-opening polymerizations, reductive coupling and other redox polymerization reactions.
Module 3 (10L)	**Inorganic Polymer Elastomers** Bridge between small and finite molecules, homopolar inorganic polymers, heteropolar inorganic polymers, Phosphorous based polymer: Polyphosphazenes, Sulphur containing polymer: Polysiloxanes, Polysilanes and Boron based polymer, Metal coordinated polymers.
Module 4 (8L)	**Applications of Inorganic Polymers** Catalysis, medical purposes, flame-retardants, high-temperature fluids and lubricants.

TEXT BOOKS/ REFERENCE BOOKS: -

- Textbook of Polymers Science, F.W. Billmeyer Jr. Wiley.
- Contemporary Polymer Chemistry, H.R. Allcock and F.W. Lambe, Prentice Hall.
- Ronald D. Archer, *Inorganic and Organometallic Polymers,* Wiley-VCH, Inc.
- James E. Mark, Harry R. Allcock, Robert West, *Inorganic polymers,* Oxford University Press, USA.
- Inorganic Chemistry, Keith F. Purcell, John C. Kotz, Cengage, India.

Lecture Plan

Lecture No.	Topics to be covered

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L1	Introduction of polymer chemistry, basic definitions
L2	Structure characteristic of the polymers
L3	Molecular weight studies and molecular weight distribution
L4 & L7	Determination of thermal parameters: DSC, TGA, DMA, TMA
L8	Mechanistic aspects
L9 & L10	Ionic, emulsion, suspension, and aqueous polymerization
L11	Classification of polymers
L12	Polymerization in homogeneous system
L13	Polymerization in heterogeneous system
L14 & L15	Step-growth polymerisation: mechanism and kinetics
L16 & L17	Chain polymerizations: mechanism and kinetics
L18 & L19	Ring-opening polymerizations: anionic, cationic and radical, Atom transfer radical polymerization
L20	Reductive coupling, Redox polymerization reactions
L21	Introduction to inorganic polymer elastomers
L22	Classification of inorganic polymers
L23 & L24	Homopolar inorganic polymers: Polyboranes and Polysilylenes
L25 & L26	Heteropolar inorganic polymers: Rings and chain molecules
L27	Phosphorous based polymer
L28	Sulphur containing polymers: Polysiloxanes, Polysilanes,
L29	Technologies of polysilanes,
L30	Boron based polymer, Metal coordinated polymers: Ferrocene based polymers

Jyoti Joshi

L31 & L32	Inorganic polymers as heterogeneous catalysts
L33 & L34	Inorganic medical polymers
L35	Polyphosphazene as biopolymer
L36	Metal based polymers for medical purposes
L37	Inorganic polymers as flame retardant
L38	Inorganic high-temperature fluids and lubricants

DETAILS OF THE COURSE

Course Type	Course Code	Course Title	Credits	Lecture	Tutorial	Practical	Studio
PC	(24CYTxxx)	Main Group Organometallic Chemistry	3	3	0	0	0

PREREQUISITE

Basic knowledge of covalent and Ionic bonds. Knowledge on the periodic properties of the elements

COURSE OBJECTIVE(s)

To impart knowledge on the bonding and structure in Main Group Organometallic compounds and recent development in their potential applications

COURSE OUTCOMES:

CO 1	Recent development of bonding and structure in main group elements
CO 2	Unusual structure and bonding in Main group elements
CO 3	Applications of earth abundant elements in catalysis

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COURSE ASSESSMENT

The Course Assessment (culminating to the final grade) will be made up of the following three components;

S. No.	Component	Weightage
1.	Internal assessment (based upon assignments, quizzes and attendance)	20%
2.	Mid-term examination	30%
3.	End Semester Examination	50%

COURSE CONTENTS

Unit 1 (6 L)	**Basics:** Milestones in organometallic chemistry, organo-element compounds: Importance in the prospect of today's demand.
Unit 2 (6 L)	**Organometallic compounds of Alkali and Alkaline-Earth Metal**: Organo-lithium compounds –Li NMR Spectroscopy. Organometallic compounds of the heavier alkali metals. Organo-beryllium, - magnesium, - calcium, - strontium and -barium compounds. Examples of some organo-zinc compounds. Some catalytic applications of Organo-magnesium and organo-zinc compounds – Synthesis of value-added chemicals.
Unit 3 (9 L)	**Organometallic Compounds of Boron group**: Organo-Boron, -aluminium, -gallium and –indium compounds. Al^{III}, Ga^{III} and In^{III} organyls and their Lewis base adducts. Chemistry of Frustrated Lewis pairs, Heterocyclic cleavage of hydrogen. Application in bulk synthesis of high value materials.
Unit 4 (9 L)	**Organo-element Compounds of Carbon Group:** Organosilicon compounds, Silicones, Silicon organometallic materials - High stability, degradability.
Unit 5 (6 L)	**Organo-element Compounds of the Nitrogen group and Oxygen group:** E^{V} (P. As) Organyls. Different Pesticides, Fertilizer – Uses, Effect on environment. Decomposition pathway, Alternatives.

TEXT BOOKS/ REFERENCE BOOKS: -

1. Christoph Elschenbroich, Orgaometallics (Third Edition), Wiley-VCH.
2. B.D. Gupta and A. J. Elias, Basic Organometallic Chemistry (Concept, Syntheses and Applications) (Second Edition) (University Press)
3. Recent Literature

Lecture Plan

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Lecture No.	Topics to be covered
1	Background and history of organometallic Chemistry – Special emphasis on main group organometallic compounds
2	Classification and discussion on the difference of main group organometallic chemistry and transition metal organometallic chemistry
3	Discussion on energy - stability, polarity and reactivity of M-C bonds - importance
4	Continued discussion on energy, polarity and reactivity with examples - importance
5	Discussion on the synthesis and structures of organo-lithium compounds. Comparison with organo-sodium compounds
6	Discussion on the reactivity - use of organo-lithium and organo-sodium compounds
7	Continued discussion on the use of organo-lithium and organo-sodium compounds, Lithium NMR
8	Discussion on organo-beryllium and organo-magnesium compounds, toxicity of beryllium.
9	Discussion on Grignard reagents – synthesis and applications. Applications of other organo-magnesium compound
10	Discussion on the recent development on the organometallic compounds of calcium, strontium and barium
11	Discussion on some related organo-zinc compounds-discussion on similarities
12	Summarization on our learning and future new chemistry
13	Discussion on the synthesis of organo-aluminium, -gallium, -indium compounds – special attention to the hydrides of all the elements
14	Discussion on the nature of the M-H bonds and their reactivity – Reducing properties of the M-H bond
15	Discussion on the Lewis acidity of the organo-aluminium, -gallium, -indium compounds and attainment of stability via adduct formation with Lewis base
16	Discussion Organo-aluminium hydroxide, aluminoxanes – synthesis and applications
17	Frustrated Lewis Pair Chemistry
18	Heterolytic splitting of hydrogen molecule

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19	Uses of Frustrated Lewis Pair Chemistry
20	Uses of Frustrated Lewis Pair Chemistry
21	Uses of Frustrated Lewis Pair Chemistry
22	Future direction in the uses of Frustrated Lewis Pair Chemistry
23	Future direction in the uses of Frustrated Lewis Pair Chemistry
24	Summarization on our learning
25	Organo-silicon compounds with coordination number 4 – synthesis and reactivity
26	Organo-silicon compounds with coordination number 3, 2, 1 and their reactivity
27	Properties and Uses of Silicon Oils
28	Different Polymers of Silicones
29	Future direction in Silicon uses
30	Summarization on our learning
31	Discussion on synthesis, structure and geometry of Ev (E = P, As, Sb) organyls
32	Discussion on synthesis, structure and geometry of Ev (E = P, As, Sb) organyls
33	Nitrogen based fertilizer and pesticides
34	Phosphorous based fertilizer and Pesticides
35	Environmental consequences of phosphorous based fertilizer
36	Summarization on our learning

DETAILS OF THE COURSE

Course Type	Course Code	Course Title	Credits	Lecture	Tutorial	Practical	Studio
PC	24CYTXX X	Bio-Inorganic Chemistry	3	3	0	0	0

PREREQUISITE

Basic knowledge of Chemistry

COURSE OBJECTIVE(s)

d) To enable the students to understand the structure, bonding, and reaction mechanism involved in the biological, bioinorganic complexes.

e) To facilitate the student to apply the practical aspects of bio-inorganic chemistry in basic and advanced research and development.
f) To understand the basic need of bio-inorganic chemistry in industrial applications.

COURSE OUTCOMES:

CO 1	Understand the importance of minerals for living organisms.
CO 2	Understand role of iron, copper, zinc etc. containing biological molecules
CO 3	Understand the applications of Bioinorganic chemistry such as in chemotherapy, imaging and other similar applications
CO 4	Explain the reaction mechanism of different metal complex reactions.
CO 5	Become familiar with the various transition metal-based inorganic materials.

COURSE ASSESSMENT

The Course Assessment (culminating to the final grade) will be made up of the following three components;

S. No.	Component	Weightage
1.	Internal assessment (based upon assignments, quizzes and attendance)	20%
2.	Mid-term examination	30%
3.	End Semester Examination	50%

COURSE CONTENTS

Course Content	
Module 1 (8L)	**Transition metal ions in Biology** Metallo-biomolecules, electron carriers, oxygen carriers and enzymes, Biogeoinorganic chemistry - environment, their occurrence and function, active- site structure and function of metallo-proteins and metallo-enzymes with various transition metal ions and ligand systems.
Module 2 (14L)	Transport and storage of Dioxygen: Heme proteins and oxygen uptake, and their coordination geometry, electronic structure and functions of hemoglobin, myoglobin and characterization of O2 bound species by

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	Raman and infrared spectroscopic methods, representative synthetic models of heme- and non- heme systems, hemocyanins and hemerythrin, model synthetic complexes of iron, copper and cobalt etc. Zinc enzymes-carboxypeptidase and carbonic anhydrase, Iron enzymes-catalase, peroxidase and cytochrome P-450, Metallo enzyme-II Copper enzymes-superoxide dismutase, Molybdenum oxotransferase enzymes-xanthine oxidase, Coenzyme vitamin B12
Module 3 (6L)	Calcium in Biology - Ion channels in biomembrane, calcium in living cells, transport and regulation, molecular, aspects of intramolecular processes, extracellular binding proteins
Module 4 (8L)	Metals in medicine, metal deficiency and disease, toxic effects of metals (Cd, Hg and Cr toxic effects with specific examples), metals used for diagnosis and chemotherapy with particular reference the anticancer drugs and MRI (Mn and Fe) agents

TEXT BOOKS/ REFERENCE BOOKS: -

a) Principles of Bioinorganic Chemistry, S. J. Lippard and J. M. Berg, University Science Books, Mill Valley, 1994.
b) Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, W. Kaim and B. Schwederski, John Wiley & Sons Inc., 1994.

Lecture Plan

Lecture No.	Topics to be covered
1 & 2	Metallo-biomolecules, electron carriers, oxygen carriers and enzymes
3 & 4	Biogeoinorganic chemistry - environment, their occurrence and function, active- site structure
5 to 8	function of metallo-proteins and metallo-enzymes with various transition metal ions and ligand systems
9 & 10	Transport and storage of Dioxygen: Heme proteins and oxygen uptake, and their coordination geometry,
11	electronic structure and functions of hemoglobin, myoglobin
12 & 13	characterization of O2 bound species by Raman and infrared spectroscopic methods
14 & 15	representative synthetic models of heme- and non- heme systems, hemocyanins and hemerythrin
16 & 17	model synthetic complexes of iron, copper and cobalt etc.
18	Zinc enzymes-carboxypeptidase and carbonic anhydrase
19	Iron enzymes- catalase, peroxidase and cytochrome P-450,
20	Metallo enzyme-II Copper enzymes-superoxide dismutase, Molybdenum oxotransferase
21 & 22	enzymes- xanthine oxidase, Coenzyme vitamin B12

Jyoti Joshi

23 & 24	Calcium in Biology - Ion channels in biomembrane
25 & 26	Calcium in living cells, transport and regulation,
27 & 28	Molecular aspects of intramolecular processes, extracellular binding proteins
29	Metals in medicine,
30	metal deficiency and disease
31 & 32	toxic effects of metals (Cd, Hg and Cr toxic effects with specific examples)
33 & 34	metals used for diagnosis and chemotherapy with particular reference the anticancer drugs
35 & 36	MRI (Mn and Fe) agents

DETAILS OF THE COURSE

Course Type	Course Code	Course Title	Credits	Lecture	Tutorial	Practical	Studio
Elective	24CYTxxx	Symmetry and Group Theory	3	3	1	0	0

PREREQUISITE

Basic knowledge of structure and bonding of inorganic compounds and coordination compounds

COURSE OBJECTIVE(s)

To impart the knowledge of symmetry and group theory in inorganic/organic compounds and its applications in various molecular spectroscopy

COURSE OUTCOMES:

CO 1	Basic knowledge of structure and geometry as per symmetry point of view
CO 2	Derivation of point group in various structures and general molecules, shapes, polygons
CO 3	Understanding of character table and its its fundamental in various spectroscopy

COURSE ASSESSMENT

The Course Assessment (culminating to the final grade) will be made up of the following three components;

S. No.	Component	Weightage
a)	Internal assessment (based upon assignments, quizzes and attendance)	20%
b)	Mid-term examination	30%
c)	End Semester Examination	50%

COURSE CONTENTS

Module 1 (6L)	**Introduction** Concept of symmetry, symmetry in nature, polygons, pyramids, prism, concept of symmetry in molecules - Symmetry operation, rotational axis of symmetry, plane of symmetry, improper axis of rotation, centre of symmetry and inversion centre, identity and determinations of various symmetry elements.
Module 2 (5L)	**Molecular Point Group** Schonfilies symbols, identification of molecular point group, cyclic point group, dihedral point group, improper point groups, molecules with special point group, molecules of high symmetry.
Module 3 5)	**Properties of Group** Properties of group, sub-group, abelian and non-abelian group, class and order of the group, matrices representations of groups.
Module 4 (10L)	**Representations, Character Table and its applications** Representations, reducible and irreducible representations, derivation of reducible representation by 3N system and bond vector method
Module 4 (10L)	**Character Table and its applications** Structure of character table, the great orthogonality theorem (without proof) and its importance, derivation of character tables for water and ammonia molecule, Mullikan symbols determination for translations and rotations, applications of group theory in FTIR and Raman and spectroscopy, molecular hybridization and NMR spectroscopy

Module 6 (2L)	**Direct product** Concept of direct product and its application in spectroscopy

TEXT BOOKS/ REFERENCE BOOKS: -

1. Physical methods in Chemistry, R. S Drago, Saunders college
2. K. Veera Reddy, Symmetry and spectroscopy of molecules, New Age Science. 2009
3. Chemical application of group theory, F. A Cotton
4. Group Theory in Chemistry, M. S. Gopinathan and V. Ramakrishnan, Vishal Publishing Co., 2nd edition.

Lecture Plan

Lecture No.	Topics to be covered
1	Concept of symmetry,
2	symmetry in nature,
3	symmetry in polygons, pyramids, prism, concept of symmetry in molecules
4	Symmetry operation, Rotational axis of symmetry, plane of symmetry,
5	Improper axis of rotation, centre of symmetry and inversion centre, identity
6	Determinations of various symmetry elements.
7	Schonfilies symbols, identification of molecular point group,
8	identification of molecular point group,
9	cyclic point group,
10	dihedral point group, improper point groups,
11	molecules with special point group, molecules of high symmetry.
12	Properties of group,
13	Properties of sub-group,

14	abelian and non-abelian group,
15	class and order of the group,
16	matrices representations of groups.
17	Reducible Representations,
18	Irreducible representations,
19	derivation of reducible representation by 3N system.
20	derivation of reducible representation by and bond vector method
21	Structure of character table, the great orthogonality theorem (without proof) and its importance, derivation of character tables for water and ammonia molecule, Mullikan symbols determination for translations and rotations, applications of group theory in FTIR and Raman and spectroscopy, molecular hybridization and NMR spectroscopy
22	the great orthogonality theorem (without proof) and its importance,
23	Examples of Green Synthesis-Ibuprofen. Industrial Green Improvements of Consumer Products
24	derivation of character tables for water
25	derivation of character tables for ammonia molecule,
26	Mullikan symbols
27	determination for translations and rotations mode of vibration
28	applications of group theory in FTIR spectroscopy,
29	applications of group theory in Raman spectroscopy,
30	molecular hybridization of water and NMR spectroscopy
31	molecular hybridization of ammoni and ironpetacarbonyl
32-35	Concept of direct product and its application in spectroscopy

DETAILS OF THE COURSE

Course Type	Course Code	Course Title	Credits	Lecture	Tutorial	Practical	Studio
PC	24CYTXXX	Organic Synthesis	3	3	0	0	0

PREREQUISITE

Basic knowledge of General Organic Chemistry

COURSE OBJECTIVE(s)

To impart knowledge of stereochemistry, reactive intermediates, mechanism of general organic reactions and Common organic reactions and rearrangements.

COURSE OUTCOMES:

CO1	Identify and differentiate prochirality and chirality at centers, axis, planes and helices and determine the absolute configuration
CO2	Analyze the role of reactive intermediates and demonstrate effect of structure on reactivity and predict the mechanism of reactions.
CO3	Gain insights into mechanistic and stereochemical features of reactions and relate the Thermodynamic and kinetic stability.

COURSE ASSESSMENT

The Course Assessment (culminating to the final grade) will be made up of the following three components;

S. No.	Component	Weightage
	Internal assessment (based upon assignments, quizzes and attendance)	20%
	Mid-term examination	30%
	End Semester Examination	50%

COURSE CONTENTS

Module 1 (10L)	**Introduction to Stereochemistry** Chirality, Isomerism, Basic concepts and principles in Stereochemistry, Methods of resolution of isomers.
Module 2	**Understanding the Structure and Reactivity in Organic Reaction**

(12L)	**Mechanism** Reactive intermediates; Generation, structure, stability and reactivity of carbocation, carbanions, free radicals, carbenes, and nitrenes. Mechanistic aspects of Thermodynamic and kinetic control, Hammond's postulate, Curtin-Hammett principle, potential energy diagrams, transition state and intermediates, methods of determining mechanisms, isotopic labeling.
Module 3 (6L)	**Reaction mechanism: Structural Effects on Stability and Reactivity** Effects of structure on reactivity, resonance and field effects, steric effects, quantitative treatment. The Hammett equation and linear free energy relationship, substituent and reaction constants, Taft equation.
Module 4 (12L)	**Selected Organic Reactions and Rearrangements** A detailed mechanistic study of the following rearrangements. Pinacol-pinacolone, Wagner-Meerwein, Demjanov, Benzil-Benzillic acid. Favorskii, Arndt-Eister synthesis, Neber, Beckmann, Hofmann, Curtius, Schmidt, Baeyer-Villiger.

(No. of lectures- 40)

TEXT BOOKS/ REFERENCE BOOKS: -

a) Advanced Organic Chemistry, Reactions Mechanisms and Structure, J. March. John Wiley.
b) Advanced Organic Chemistry, F.A. Carey and R.J. Sunderg, Plenum.
c) A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.
d) Structure and Mechanism in Organic Chemistry, C.K. Ingold, Cornell University Press.
e) Modern Synthetic Reactions. H.O. House, W.A. Benjamin.
f) Some Modern Methods of Organic Synthesis, W. Carruthers, Cambridge Univ. Press.
g) Principles of Organic synthesis, R.O.C. Norman and J.M. Coxon, Blackie Academic & Professional.

Lecture Plan

Lecture No.	Topics to be covered
1-3	Stereochemistry-Introduction, basic concepts and principles in stereochemistry, fundamentals of elements of symmetry.
4-6	Chirality-Basic concept, optical activity, configuration of chiral molecules (relative configuration-D/L system and absolute configuration- R/S system) and Threo and erythron isomers wrt to optical activity.
7-10	Projection formulae- (i) Fischer (ii) Sawhorse (iii) Newman (iv) Flying Wedge and their interconversions, enantiotopic and diastereotopic atoms, and Methods of resolution of isomers.
11-16	Reactive intermediates; Generation, structure, stability and reactivity of carbocation, carbanions, free radicals, carbenes, nitrenes
17-20	Mechanistic aspects of Thermodynamic and kinetic control. Thermodynamic and kinetic requirements. Hammond's postulate, Curtin-Hammett principle. Potential energy diagrams, transition state and intermediates.

21-22	Methods of determining mechanisms, Isotopic (Deuterium) effect and isotopic labeling.
23-26	Effects of structure on reactivity, resonance and field effects, steric effects, quantitative treatment.
27-28	The Hammett equation and linear free energy relationship, substituent and reaction constants. Taft equation.
29-32	A detailed mechanistic study of Pinacol-pinacolone Wagner-Meerwein, Demjanov and Benzil-Benzillic acid rearrangements involving carbocation.
33-35	Arndt-Eister synthesis and wolf rearrangements, Favorskii reaction/rearrangements, Baeyer-Villiger oxidation and rearrangements.
36-40	Hofmann, Curtius, Schmidt rearrangements, Neber and Beckmann rearrangements with mechanism and examples.

DETAILS OF THE COURSE

Course Type	Course Code	Course Title	Credits	Lecture	Tutorial	Practical	Studio
PC	24CYTXXX	Applied Bio-catalysis (Enzymes)	3	3	0	0	0

PREREQUISITE

Basics of enzyme catalysis

COURSE OBJECTIVE(s)

To impart the knowledge of biological reactions including enzyme catalysis in different reactions.

COURSE OUTCOMES:

CO1	Understand the theories of enzyme kinetics in the cell
CO2	Mechanisms of enzyme catalysis, and the mechanisms of enzyme regulation in the cell
CO3	Describe and use the equations of enzyme kinetics.

COURSE ASSESSMENT

The Course Assessment (culminating to the final grade) will be made up of the following three components;

S. No.	Component	Weightage
	Internal assessment (based upon assignments, quizzes and attendance)	20%

	Mid-term examination	30%
	End Semester Examination	50%

COURSE CONTENTS

Module 1 (4L)	**Introduction** Nature of enzymes - protein and non-protein (ribozyme). Cofactor and prosthetic group. Nomenclature and classification.
Module 1 (12L)	**Enzymes** Factors affecting the rate of chemical reactions, collision theory, activation energy and transition state theory, catalysis, reaction rates and thermodynamics of reaction. Catalytic power and specificity of enzymes (concept of active site), Fischer's lock and key hypothesis, Koshland's induced fit hypothesis. Relationship between initial velocity and substrate concentration, steady state kinetics, equilibrium constant- monosubstrate reactions. Michaelis-Menten equation, Lineweaver Burk plot. Km and Vmax, Kcat and turnover number.
Module 1 (8L)	**Mechanism of Enzyme Action** General features - proximity and orientation, strain and distortion, acid base and covalent catalysis. Examples of some typical enzyme mechanisms for chymotrypsin, ribonuclease, lysozyme and carboxypeptidase.
Module 1 (8L)	**Reactions Catalyzed by Enzymes** Nucleophilic displacement on a phosphorus atom, multiple displacement reactions and the coupling of ATP cleavage to endergonic processes. Transfer of sulphate, addition and elimination reactions, enolic intermediates in Isomerization's reactions, α-Cleavage and condensation, some isomerization and rearrangement reactions. Enzyme catalyzed carboxylation and decarboxylation.
Module 1 (8L)	**Applications of Enzymes** Techniques and methods of immobilization of enzymes, effect of immobilization on enzyme activity, application of immobilized enzymes, use of enzymes in food and drink industry-brewing and cheese-making, syrups from corn starch, enzymes as targets for drug design. Clinical uses of enzymes, enzyme therapy, enzymes and recombinant DNA Technology.

(No. of lectures- 40)

TEXT BOOKS/ REFERENCE BOOKS: -

a) Bioorganic Chemistry: A Chemical Approach to Enzyme Action, Hermann Dugas and C. Penny, Springer Verlag.
b) Understanding Enzymes, Trevor Palmer, Prentice Hall.
c) Enzyme Chemistry: Impact and applications, Ed. Collin J suckling, chemistry.Enzyme Mechanisms Ed. M.I. Page and A Williams, Royal Society of Chemistry.
d) Fundamentals of Enzymology, N.C. Price and L. Stevens. Oxford University Press.
e) Immobilized Enzymes: An Introduction and Applications in Biotechnology, Michael ID. Trevan, John Wiley.
f) Enzymatic Reaction Mechanisms. C. Walsh. W.H. Freeman.
g) Enzyme Structure and Mechanism, A Fersht, W.H. Freeman.
h) Biochemistry: The Chemical Reactions of Living Cells, D.E. Metzler, Academic Press.

Lecture Plan

Lecture No.	Topics to be covered
1-2	Nature of enzymes - protein and non-protein (ribozyme). Cofactor and prosthetic group.
3-4	Nomenclature and classification.
5-8	Factors affecting the rate of chemical reactions and Collision theory and activation energy. Transition state theory Catalysis, reaction rates and thermodynamics of reaction.
9-12	Catalytic power and specificity of enzymes (concept of active site), Fischer's lock and key hypothesis, Koshland's induced fit hypothesis
13-16	Relationship between initial velocity and substrate concentration, steady state kinetics equilibrium constant - monosubstrate reactions Michaelis-Menten equation, Lineweaver Burk plot. Km and Vmax, Kcat and turnover number.
17-20	General features - proximity and orientation, strain and distortion, acid base and covalent catalysis.
21-24	Examples of some typical enzyme mechanisms for chymotrypsin, ribonuclease, lysozyme and carboxypeptidase.
25-28	Nucleophilic displacement on a phosphorus atom, multiple displacement reactions and the coupling of ATP cleavage to endergonic processes. Transfer of sulphate, addition and elimination reactions,
29-32	Enolic intermediates in Isomerization's reactions, a-Cleavage and condensation, some isomerization and rearrangement reactions. Enzyme catalyzed carboxylation and decarboxylation.
33-36	Techniques and methods of immobilization of enzymes, effect of immobilization on enzyme activity, application of immobilized enzymes.
37-40	Use of enzymes in food and drink industry-brewing and cheese-making, syrups from corn starch, enzymes as targets for drug design. Clinical uses of enzymes, enzyme therapy, enzymes and recombinant DNA Technology.

Jyoti Joshi

DETAILS OF THE COURSE

Course Type	Course Code	Course Title	Credits	Lecture	Tutorial	Practical	Studio
PC	24CYTXXX	Heterocyclic Chemistry	3	3	0	0	0

PREREQUISITE

None

COURSE OBJECTIVE(s)

Heterocyclic compounds are very interesting due to their distinct structure and their availability in Nature and in Medicinal Drugs. So, the technique of synthesis of heterocyclic compounds is important in the synthesis of different drugs. This course gives quantitative ideas about the synthesis, properties and uses of such heterocyclic compounds.

COURSE OUTCOMES:

CO1	Explain nomenclature, synthesis and reactivity of three, five and six membered heterocyclic compounds
CO2	Explain various methods of ring synthesis, reactivity and applications of heterocyclic compounds and their derivatives.
CO3	Acquire knowledge on various biosynthetic pathways.

COURSE ASSESSMENT

The Course Assessment (culminating to the final grade) will be made up of the following three components;

S. No.	Component	Weightage
	Internal assessment (based upon assignments, quizzes and attendance)	20%
	Mid-term examination	30%
	End Semester Examination	50%

COURSE CONTENTS

Module 1 (4L)	**Structure and Systematic Nomenclature of Heterocycles Compounds**
Module 2 (12L)	**Three- Membered Heterocyclic Compounds-** Synthesis and reactions including medicinal applications of Oxirane, Aziridine, Dioxirane, Oxaziridine, 3H-Diazirine, Diaziridine.

Module 3 (8L)	**Five-Membered Heterocyclic Compounds** Synthesis and reactions including medicinal applications of Furan, Thiophene, Pyrrole, Indole, benzopyrroles, bezofurans and benzothiophenes
Module 4 (8L)	**Six-Membered Heterocycles** Synthesis and reactions of pyrylium salts and pyrones and their comparison with pyridinium & thiopyrylium salts and pyridones. Synthesis and reactions of quinolizinium and benzopyrylium salts, coumarins and chromones.
Module 4 (8L)	**Six Membered Heterocycles with two-Heteroatoms** Synthesis and reactions of diazines and triazines. Seven-and Large-Membered Heterocycles- Synthesis and reactions of azepines, oxepines and thiepines.

(No. of lectures- 40)

TEXT BOOKS/ REFERENCE BOOKS: -

4. Heterocyclic Chemistry Vol. 1-3, R.R. Gupta, M. Kumar and V. Gupta, Springer Verlag
5. The Chemistry of Heterocycles, T. Eicher and S. Hauptmann, Thieme
6. Heterocyclic chemistry J.A. Joule, K. Mills and g. F. Smith, Chapman and Hall
7. Heterocyclic Chemistry, T.L. Gilchrist, Longman Scientific Technical
8. Contemporary Heterocyclic Chemistry, G. R. Newkome and W.W. Paudler, Wiley-Inter Science
9. An Introduction to the Heterocyclic Compounds, R.M. Acheson, John Wiley
7. Comprehensive Heterocyclic Chemistry, A.R. Katritzky and C.W. Rees, eds. Pergamon Press

Lecture Plan

Lecture No.	Topics to be covered
1-4	Structure and Systematic Nomenclature of Heterocycles Compounds
5-8	Synthesis and reactions including medicinal applications of Oxirane, Aziridine
9-12	Synthesis and reactions including medicinal applications of Dioxirane, Oxaziridine
13-16	Synthesis and reactions including medicinal applications of 3H-Diazirine, Diaziridine
17-20	Synthesis and reactions including medicinal applications of Furan, Thiophene, Pyrrole
21-24	Indole, benzopyrroles, bezofurans and benzothiophenes
25-28	Synthesis and reactions of pyrylium salts and pyrones and their comparison with pyridinium & thiopyrylium salts and pyridones..
29-32	Synthesis and reactions of quinolizinium and benzopyrylium salts, coumarins and chromones
33-36	Synthesis and reactions of diazines and triazines.
37-40	Seven-and Large-Membered Heterocycles- Synthesis and reactions of azepines, oxepines and thiepines.

DETAILS OF THE COURSE

Course Type	Course Code	Course Title	Credits	Lecture	Tutorial	Practical	Studio
PC	24CYTXXX	Cell Structure and Biomolecules	3	3	0	0	0

PREREQUISITE

None

COURSE OBJECTIVE(s)

This course includes basic knowledge of biology including cell structure, molecules of life (Biomolecules) such as carbohydrates, lipids, amino acids, protein.

COURSE OUTCOMES:

CO 1	Understand the basics of cell and its components
CO 2	Understand the foundation on the basic module of life
CO 3	Understand the structure, properties and biosynthesis of important biomolecules like carbohydrates, lipids and proteins.

COURSE ASSESSMENT

The Course Assessment (culminating to the final grade) will be made up of the following three components;

S. No.	Component	Weightage
g)	Internal assessment (based upon assignments, quizzes and attendance)	20%
h)	Mid-term examination	30%
i)	End Semester Examination	50%

COURSE CONTENTS

Course Content	
Module 1 (10L)	Structure of prokaryotic and eukaryotic cell. Intracellular organelles and their function, comparison of plant and animal cells. Overview of metabolic processes – catabolism and anabolism. ATP the biological energy currency. Origin of life -unique properties of carbon, chemical evolution and rise of living systems. Introduction to Biomolecules, building blocks of bio macromolecules.
Module 2 (6L)	Structure and function of carbohydrates: mono-, di-, oligo- and poly-saccharides
Module 3 (10L)	Fatty acids, essential fatty acids. Structure and function of diglycerols, glycerophospholipids. Sphingolipids, cholesterol, bile acids, prostaglandins. Lipoproteins composition and function. Properties of lipid aggregate-micelles, bilayers, liposomes and their possible biological functions, biological membranes. Fluid mosaic model of membrane structure. Lipid metabolism, β-oxidation of fatty acids.
Module 4 (10L)	Chemical and enzymatic hydrolysis of properties to peptides, amino acid sequencing. Secondary structure of proteins, forces responsible for holding of secondary structure α-helix, β-sheets, super secondary structure, triple helix structure of collagen. Tertiary structure of protein-folding and domain structure. Quaternary structure. Amino acid metabolism-degradation and biosynthesis of amino acids, sequence determination: chemical/enzymatic/mass spectral, racemization/detection. Chemistry of oxytocin and tryptophan releasing hormone (TRH)

TEXT BOOKS/ REFERENCE BOOKS: -

1. Nelson DL and Cox MM; Lehninger principles of biochemistry, Sixth edition, WH Freeman and company, 2012
2. Berg JM, Tymoczko JL and Stryer L; Biochemistry, Seventh edition, WH Freeman and company, 2011
3. Voet D and Voet JG; Biochemistry, Fourth edition, John Wiley and Sons, 2011
4. Pelczar MJ, Chan ECS and Krieg NR; Microbiology, Tata McGraw-Hill, Fifth edition, 2008 (37Th reprint)

Lecture Plan

Lecture No.	Topics to be covered

Jyoti Joshi

1	Structure of prokaryotic and eukaryotics cell
2	comparison of plant and animals cells
3	Intracellular organelles and their function
4	
5	Overview of metabolic processes – catabolism and anabolism, ATP the biological energy currency
6	
7	Origin of life -unique properties of carbon, chemical evolution and rise of living systems
8	
9	Introduction to Biomolecules, building blocks of bio macromolecules.
10	
11	Structure of carbohydrates
12	
13	Types of Polysaccharides: mono-, di-, oligo- and poly- saccharides
14	
15	Function of carbohydrates
16	
17	Fatty acids, essential fatty acids.
18	Structure and function of diglycerols, glycerophospholipids.
19	Sphingolipids, cholesterol, bile acids, prostaglandins
20	
21	Lipoproteins composition and function
22	Properties of lipid aggregate-micelles, bilayers, liposomes and their possible biological functions
23	
24	Biological membranes. Fluid mosaic model of membrane structure.
25	Lipid metabolism, β-oxidation of fatty acids.
26	
27	Amino acids and peptide bond.
28	Chemical and enzymatic hydrolysis of properties to peptides, amino acid sequencing
29	Secondary structure of proteins, forces responsible for holding of secondary structure α-helix, β-sheets,
30	super secondary structure, triple helix structure of collagen
31	Tertiary structure of protein-folding and domain structure.
32	Quaternary structure
33	Amino acid metabolism-degradation and biosynthesis of amino acids,
34	sequence determination: chemical/enzymatic/mass spectral, racemization/detection.
35	
36	Chemistry of oxytocin and tryptophan releasing hormone (TRH)

DETAILS OF THE COURSE

Course Type	Course Code	Course Title	Credits	Lecture	Tutorial	Practical	Studio
PC	24CYTXXX	Biochemistry	3	3	0	0	0

PREREQUISITE

None

COURSE OBJECTIVE(s)

This course examines the chemical and physical properties of the building blocks of cell, with special emphasis on the structures of proteins and nucleic acids, their roles in propagation of genetic codes, roles of enzymes in catalyzing biochemical processes and basic principles of metabolism.

COURSE OUTCOMES:

CO 1	Introduction to the chemical processes of life: Their structures, chemistry and functions
CO 2	Gain basic ideas about the flow of genetic codes via chemical transformation occurring inside cells
CO 3	Understand the role of enzymes in realizing complex chemical reactions under mild conditions
CO 4	Introduction to the central pathways of metabolism and understanding the associated chemical transformations involved therein

COURSE ASSESSMENT

The Course Assessment (culminating to the final grade) will be made up of the following three components;

S. No.	Component	Weightage
1.	Internal assessment (based upon assignments, quizzes and attendance)	20%
2.	Mid-term examination	30%
3.	End Semester Examination	50%

COURSE CONTENTS

Course Content	
Module 1 (10L)	**Proteins** Primary structure: Amino acids, peptide bonds, polypeptide chain's Secondary structure: α -helices, parallel and antiparallel β-sheets, β-turns, γ-turns, Ramachandran plot Tertiary structure: Protein folding, Levinthal's paradox, Motifs and domains, Protein sequencing and structure determination: Mass & NMR spectroscopy, X-ray crystallography, Protein misfolding and related disease.
Module 2 (10L)	**Nucleic acids** Nucleobases, nucleosides and nucleotides, Single stranded RNA, Double helix DNA, A, B and Z-DNA structures, DNA replication: polymerases, Transcription: mRNA, reverse transcription, Translation: codon, role of tRNA and ribosome, Genomes, genes, Polymerase chain reaction (PCR), Use of modified bases in PCR, mutagenesis (random and site directed), recombinant DNA technology and its use
Module 3 (6L)	**Enzymes and their kinetics** Enzymes as Catalysts: role of cofactors, active sites and enzyme-substrate complex Michaelis-Menten kinetics and its extension, competitive, Inhibition of enzymes: reversible (competitive, uncompetitive and noncompetitive) and irreversible. Effect of pH and temperature on enzyme activity
Module 4 (10L)	**Metabolism** ATP: Universal currency of free energy, ATP hydrolysis, Glycolysis and gluconeogenesis, Krebs cycle, Oxidative phosphorylation, Photosynthesis, Calvin cycle, Pentose phosphate pathway

TEXT BOOKS/ REFERENCE BOOKS: -

1. Nelson DL and Cox MM; Lehninger principles of biochemistry, Sixth edition, WH Freeman and company, 2012
2. Berg JM, Tymoczko JL and Stryer L; Biochemistry, Seventh edition, WH Freeman and company, 2011
3. Voet D and Voet JG; Biochemistry, Fourth edition, John Wiley and Sons, 2011
4. Pelczar MJ, Chan ECS and Krieg NR; Microbiology, Tata McGraw-Hill, Fifth edition, 2008 (37Th reprint)

Jyoti Joshi

Lecture Plan

Lecture No.	Topics to be covered
1	Primary structure: Amino acids, peptide bonds, polypeptide chain's
2	
3	Secondary structure: α -helices,
4	parallel and antiparallel β-sheets, β-turns, γ-turns
5	
6	Ramachandran plot
7	Tertiary structure: Protein folding, Levinthal's paradox,
8	Motifs and domains, Protein sequencing
9	structure determination: Mass & NMR spectroscopy, X-ray crystallography
10	Protein misfolding and related disease.
11	Nucleobases, nucleosides and nucleotides,
12	Single stranded RNA
13	Double helix DNA, A, B and Z-DNA structures,
14	DNA replication: polymerases,
15	Transcription: mRNA, reverse transcription,
16	Translation: codon,
17	role of tRNA and ribosome,
18	Genomes, genes, Polymerase chain reaction (PCR),
19	Use of modified bases in PCR, mutagenesis (random and site directed), recombinant DNA technology and its uses
20	
21	Enzymes as Catalysts: role of cofactors, active sites and enzyme-substrate complex
22	
23	Michaelis-Menten kinetics and its extension, competitive,
24	Inhibition of enzymes: reversible (competitive, uncompetitive and noncompetitive) and irreversible.
25	
26	Effect of pH and temperature on enzyme activity
27	ATP: Universal currency of free energy, ATP hydrolysis
28	Glycolysis and gluconeogenesis,
29	
30	Krebs cycle,
31	
32	Oxidative phosphorylation,
33	
34	Photosynthesis, Calvin cycle,
35	
36	Pentose phosphate pathway

DETAILS OF THE COURSE

Course Type	Course Code	Course Title	Credits	Lecture	Tutorial	Practical	Studio
PC		Physical Organic Chemistry	3	3	0	0	0

PREREQUISITE

None

COURSE OBJECTIVE(s):

This course will connect the knowledge of physical chemistry to traditional organic synthesis and mechanism.

COURSE OUTCOMES:

CO 1	To connect the physical chemistry knowledge to the organic synthesis and mechanism.
CO 2	invoke known mechanisms and intermediates to explain observed chemical phenomena

COURSE ASSESSMENT

The Course Assessment (culminating to the final grade) will be made up of the following three components;

S. No.	Component	Weightage
1.	Internal assessment (based upon assignments, quizzes and attendance)	20%
2.	Mid-term examination	30%
3.	End Semester Examination	50%

COURSE CONTENTS

Module 1 [Lectures: 5] Description of molecules: (includes reactive intermediates as radicals, carbenes, carbocations and carbanions) based on the Quantum mechacanical valence bond theory and molecular orbital theory.

Module 2 [Lectures: 6] Conformational analysis of organic molecules: NMR analysis of hindered rotation (determination of the rate constant at the coalescence temperature), energy-reaction coordinate diagram for simultaneously rotation of two C-C bonds and a short introduction to molecular mechanic calculations.

Module 3 [Lectures: 18] Energy surfaces (2D and 3D) and kinetic analyses in the study of reaction mechanisms: Ke More O'Ferral-Jencks plot (variable transition-state diagram), reaction order and rate laws, the steady-state approximation in the study of complex reactions, kinetic versus thermodynamic control, the principle of microscopic reversibility, the Curtin-Hammett principle, the Hammonds postulate. Energy functions from rate constants and reaction temperatures: The Arrhenius (activation energy) and the Eyring (enthalpy and entropy of activation) equations. Kinetic isotope effects (primary and secondary). Polanyi' rule of mode selectivity.

Module 4 [Lectures: 08] (a) The Hammett equation for aromatic compounds, substituent and reaction constants, significance of the Hammett reaction constant values, deviations from linearity mechanistic information in multi-step reactions. (b) The Swain-Scott equation (nuclophilicity versus basicity). (c) The Grunwald-Winstein and the Schleyer equations(quantifying solvent effects and nucleophilicity).

Module 5 [Lectures: 3] Classification of solvents based on physical properties: dielectric constant, refractive index, dipole moment, donor number, acceptor number, hydrogen bond acceptor capacity alpha, hydrogen bond donor capacity beta and the Reichardt's Et scales.

Reference Books:

R1. E. V. Anslyn; D. A. Dougherty: Modern Physical Organic Chemistry (University Science Books)

R2. F. A. Carey; R. J. Sundberg: Advanced Organic Chemistry, Part A: Structure and Mechanisms (Springer)

R3. T. H. Lowry and K. S. Richardson: Mechanism and Theory in Organic Chemistry (Pearson)

Lecture Plan

Sl. No.	Lectures	Topic	Text book/ Reference book

		Module-I Description of molecules:	
		Total Lectures: 5	
	L1-L2	Introduction to valence bond concepts	R1, R2,R3
-	L3-L4	Introduction to Molecular Orbital theory concepts	R1, R2,R3
	L5-L6	Quantum Chemical description of reactive intermediates as radicals, carbenes, carbocations and carbanions	R1, R2,R3
		Assignment 1	
		Module- II Conformational analysis of organic molecules:	
		Total Lectures : 06	
-	L6-L8	NMR analysis of hindered rotation (determination of the rate constant at the coalescence temperature), and	R1, R2,R3
-	L9-L10	Energy-reaction coordinate diagram for simultaneously rotation of two C-C bonds	R1, R2,R3
	L11-L12	a short introduction to molecular mechanic calculations.	R1, R2,R3
		Assignment 2	
		Module- III Energy surfaces (2D and 3D) and reaction mechanisms::	
		Total Lectures: 18 **Total Tutorials:**	
	L13-L15	Introduction to Potential Energy surfaces	
-	L16	Ke More O'Ferral-Jencks plot (variable transition-state diagram)	R1, R2, R3
	L17-L18	reaction order and rate laws, the steady-state approximation in the study of complex reactions,	R1, R2, R3
-	L19	kinetic versus thermodynamic control,	R1, R2, R3
	L20-L22	the Curtin-Hammett principle, the Hammonds postulate.	R1, R2, R3
-	L23-L26	Energy functions from rate constants and reaction temperatures: The Arrhenius (activation energy) and the Eyring (enthalpy and entropy of activation) equations.	R1, R2, R3
	L27-L28	Kinetic isotope effects (primary and secondary)	R1, R2,R3

	L29-L30	Polanyi' rule of mode selectivity.	R1, R2,R3
		Assignment 3	
		Module- IV	
		Total Lectures: 8 **Total Tutorials:**	
-	L31	The Hammett equation for aromatic compounds	R1, R2,R3
-	L32-L33	substituent and reaction constants	R1, R2,R3
	L34	significance of the Hammett reaction constant values	R1, R2,R3
-	L35-L36	The Swain-Scott equation (nuclophilicity versus basicity).	R1, R2,R3
	L37-L38	The Grunwald-Winstein and the Schleyer equations	R1, R2,R3
		Assignment 3	
		Module- V Classification of solvents based on physical properties:	
		Total Lectures: 3 **Total Tutorials:**	
-	L39-L42	dielectric constant, refractive index, dipole moment, donor number, accept number, hydrogen bond acceptor capacity alpha, hydrogen bond don capacity beta and the Reichardt's Et scales.	

DETAILS OF THE COURSE

Course Type	Course Code	Course Title	Credits	Lecture	Tutorial	Practical	Studio
PE	24CYTXXX	Electrochemistry: Ionics and	3	3	0	0	0

		Electrodics					

PREREQUISITE:

Basic understanding of Physical Chemistry and Electrochemistry

COURSE OBJECTIVE(s):

To be able to apply theories of electrochemistry to analyze fundamental electrochemical processes in liquid as well as solid phases.

COURSE OUTCOMES:

CO 1	To represent electrochemical cell and write relevant electrochemical equations,explain potential, overpotential and thermodynamics involved during the operation of the cells
CO 2	To estimate electrochemical cell parameters and electrochemical behaviors of electrodes and electrolytes
CO 3	Understand basic electrochemical methods relevant to electrochemical energy storage

COURSE ASSESSMENT

The Course Assessment (culminating to the final grade) will be made up of the following three components:

S. No.	Component	Weightage
j)	Internal assessment (based upon assignments, quizzes and attendance)	20%
k)	Mid-term examination	30%
l)	End Semester Examination	50%

COURSE CONTENTS

Jyoti Joshi

Unit I: Electrochemical cells and reactions; faradaic and non-faradaic electrode processes; nature of electrode-solution interface in non-faradaic processes; factors effecting rates of faradaic electrode reactions; potential and basic thermodynamics of cells; equilibrium electrode potentials; liquid junction potential; selective electrodes.

(10 Hours)

Unit II: Electrode/electrolyte interface; current-potential relationship (Butler-Volmer and Tafel equations); overpotential - types, origin, and minimization; hydrogen evolution and oxygen reduction reactions; underpotential deposition of metals; potential step methods; potential sweep methods; pulse techniques; controlled current techniques; polarizable and non-polarizable electrodes, types of reference and working electrodes. **(16 Hours)**

Unit III: Interface electrical phenomena in ionic solids; defect chemistry in solid state electrochemistry; various solid electrolytes, mixed ionic-electronic conductors; experimental methods to study solid electrolytes; high-temperature solid electrolytes; important applications of solid electrolytes; future perspectives of solid electrolytes; electrochemistry for energy applications. **(10 Hours)**

TEXT BOOKS/ REFERENCE BOOKS:

- Modern Electrochemistry by J. O´M. Bockris and A.K.N Reddy, Springer 2000.
- Electrochemical Methods: Fundamentals and Applications by J. Bard and L. R Faulkner, Wiley, 2001
- Fundamentals of Electrochemistry by Vladimir S. Bagotsky. Wiley, 2005.

Lecture Plan

Lecture No.	Topics to be covered
1	Electrochemical cells and reactions
2	Faradaic electrode processes
3	Non-faradaic electrode processes
4	Nature of electrode-solution interface in non-faradaic processes
5	Factors effecting rates of faradaic electrode reactions
6	Cell potential
7	Basic thermodynamics of cells
8	Equilibrium electrode potentials

Jyoti Bashi

9	Liquid junction potential
10	Selective electrodes
11	Electrode/electrolyte interface
12	Butler-Volmer equation
13	Tafel equations
14	Overpotential: types and origin
15	Minimization of overpotential
16	Hydrogen evolution reaction
17	Oxygen reduction reactions
18	Underpotential deposition of metals
19	Potential sweep methods-I
20	Potential sweep methods-II
21	Potential sweep methods
22	Pulse electrochemical techniques
23	Controlled current techniques
24	Polarizable and non-polarizable electrodes
25	Types of reference electrodes
26	Types of working electrodes
27	Interface electrical phenomena in ionic solids
28	Defect chemistry in solid state electrochemistry
29	Various solid electrolytes
30	Mixed ionic-electronic conductors
31	Experimental methods to study solid electrolytes
32	High-temperature solid electrolytes
33	Important applications of solid electrolytes

34	Future perspectives of solid electrolytes
35	Electrochemistry for energy applications-I
36	Electrochemistry for energy applications-II

DETAILS OF THE COURSE

Course Type	Course Code	Course Title	Credits	Lecture	Tutorial	Practical	Studio
PC	24CYTXXX	Advanced Analytical Chemistry	3	3	0	0	0

PREREQUISITE

None

COURSE OBJECTIVE(s)

1. To enable the students to acquire advance knowledge of analytical techniques for various applications
2. To bring adaptability to recent developments in analytical chemistry and a knowledge of contemporary issues
3. To make them apply the knowledge of advanced analytical chemistry for identification of structures of organic molecules as well as their estimation

COURSE OUTCOMES:

CO 1	Students will be able to understand various aspects and importance of advanced analytical tools to understand their importance and applications
CO 2	Students will be able to interpret structures of compounds by the advanced working on the principles of analytical chemistry
CO 3	Students will be able to conduct investigations of complex problems by the use research-based knowledge and research methods including design of experiments, analysis and interpretation of data, and synthesis of the information to provide valid conclusions.

COURSE ASSESSMENT

Jyoti Joshi

The Course Assessment (culminating to the final grade) will be made up of the following three components;

S. No.	Component	Weightage
1.	Internal assessment (based upon assignments, quizzes and attendance)	20%
2.	Mid-term examination	30%
3.	End Semester Examination	50%

COURSE CONTENTS

Please Include details module wise along with number of lectures.

(No. of lectures- 38)

Course Content	
Unit 1(8L)	**Atomic spectrometric methods:** Principle, instrumentation and applications of atomic absorption, atomic emission and atomic fluorescence, beam modulation in AAS, spectral and chemical interferences in atomic spectroscopy, qualitative and quantitative analysis, Internal standard and standard addition calibration
Unit 2(6L)	**Liquid-liquid extraction:** Principle, significance of various terms, batch and counter current extraction, classification and details of extractants, Extraction terms emulsion formation, identification of extracting species.
Unit 3(6L)	**Radiometric and Nuclear methods of analysis:** Concept of radiotracers and radiolabelling, radioisotope production, radioactivity and radiation measurement, activation analysis, isotope dilution method, radioimmunoassay and radio reagent methods, Positron emission spectroscopy
Unit 4(6L)	**Spectral methods:** **X-ray methods**: X-ray spectra, x-ray absorption, emission, fluorescence and diffraction methods, monochromatization, detection of x-rays, application of x-ray spectroscopy for analyses and characterization of materials, Particle Induced X-ray Emission, Optical and electron microscopy.
Unit 5(10L)	**Chromatographic techniques:** Gas chromatography, high pressure liquid chromatography, instrumentation, detector characteristics, ion chromatography, size exclusion chromatography, Ion exchange and affinity chromatography, synthetic

	inorganic ion-exchangers – classification and applications, LC-MS, GC-MS, ICP-MS, MS-MS, ion sources (ESI, APCI, CI), source and compound parameters,

TEXT BOOKS/ REFERENCE BOOKS: -

1. Mendham J., Denney R.C., Barnes J.D. and Thomas M.J.K., "Vogel's Text Book of Quantitative Chemical Analysis", 6th Ed., Pearson Education. 2004
2. Skoog D.A., West D.M., Holler F.J. and Crouch S.R., "Fundamentals of Analytical Chemistry", 8th Ed., Thomson Brooks/Cole. 2004
3. Christian G.D., "Analytical Chemistry", 6th Ed., John Wiley & Sons Inc. 2004
4. Fifield F.W. and Kealey D., "Principles and Practice of Analytical Chemistry", 5th Ed., Blackwell Science. 2000
5. Mendham J., Denney R.C., Barnes J.D. and Thomas M.J.K., "Vogel's Text Book of Quantitative Chemical Analysis", 6th Ed., Pearson Education. 2004
6. Ewing G.W., "Instrumental Methods of Chemical Analysis", 5th Ed., McGraw Hill Book Company, Inc. 2004
7. Rochow T.G. and Tuckor P.A. "Introduction to microscopy by means of light, electron, X- rays or Acoustics", Springer, 2nd Ed. 2005
8. Jenkins R., "X-ray fluorescence spectrometry (Chemical Analysis; A series of Monographs on Analytical Chemistry and its application", Wiley-Interscience, 2nd Ed.) 1999

Lecture Plan

Lecture No.	Topics to be covered
1	**Unit-I Atomic Absorption Spectrometry:** Principle, instrumentation and applications of atomic absorption-I,
2	Principle, instrumentation and applications of atomic absorption-II
3	Spectral and chemical interferences in atomic spectroscopy
4	Internal standard and standard addition calibration of Instruments
5	Qualitative and quantitative analysis of various samples
6	Discussions on atomic emission and atomic fluorescence,
7	Beam modulation in AAS
8	Problems and solution discussions
9	Unit-II: **Liquid-liquid extraction:** Principle, significance of various terms
10	Information on Batch and counter current extraction

Jyoti Joshi

11	Classification and details of extractants,
12	Extraction terms emulsion formation
13	Identification of extracting species
14	Problems and solution discussions
15	Unit-III: **Radiometric and Nuclear methods of analysis:** Concept of radiotracers and radiolabelling, ,
16	radioisotope production, radioactivity and radiation measurement,
17	activation analysis, isotope dilution method,
18	radioimmunoassay and radio reagent methods
19	Positron emission spectroscopy- Introduction and basic concepts
20	Positron emission spectroscopy- Applications
21	Unit-IV: **Spectral methods:** **X-ray methods**: Introduction to X-ray spectra, Production of X-rays
22	X-ray absorption, emission, fluorescence and diffraction methods
23	Monochromatization, production and detection of x-rays,
24	Application of x-ray spectroscopy for analyses and characterization of materials
25	Particle Induced X-ray Emission
26	Optical and electron microscopy basics and applications
27	Unit-V: **Chromatographic techniques:** Introduction to chromatography, basics and understanding of various terminologies,
28	Gas chromatography, Principals, instrumentations and applications
29	High pressure liquid chromatography, instrumentation
30	Detector characteristics of various chromatography, ion chromatography, size exclusion chromatography, Ion exchange and affinity chromatography
31	synthetic inorganic ion-exchangers – classification and applications,
32	LC-MS; Principals, instrumentations and applications
33	GC-MS, Principals, instrumentations and applications
34	ICP-MS, Principals, instrumentations and applications
35	MS-MS, ion sources (ESI, APCI, CI), source and compound

	parameters,
36	MS-MS, ion sources (ESI, APCI, CI), source and compound parameters –Contd…

DETAILS OF THE COURSE

Course Type	Course Code	Course Title	Credits	Lecture	Tutorial	Practical	Studio
PC	24CYTXXX	Introduction to Astrochemistry	3	3	0	0	0

PREREQUISITE

None

COURSE OBJECTIVE(s)

The course provides an introduction to the knowledge of the underlying theory and methods of various types of spectroscopy encompassing a large window of the electromagnetic spectrum starting from radio wave to X-ray

COURSE OUTCOMES:

CO 1	Understand the nature and underlying physical laws of interaction between molecules and electromagnetic radiation
CO 2	Know the various factors responsible for the spectral shapes we observe
CO 3	Gain fundamental information on how different molecular motions results in different spectroscopic methods
CO 4	Select molecular spectroscopy methods suitable for solving given scientific problem
CO 5	Analyze measured spectra to shed light on the structure, activity of the molecule as well as the environment and physical conditions

COURSE ASSESSMENT

The Course Assessment (culminating to the final grade) will be made up of the following three components;

Jyoti Joshi

S. No.	Component	Weightage
1.	Internal assessment (based upon assignments, quizzes and attendance)	20%
2.	Mid-term examination	30%
3.	End Semester Examination	50%

COURSE CONTENTS

Unit 1 **(6L)**	**1. Matter and radiation:** Classical and quantum theory of light, absorption and emission of radiation by molecular species, Einstein A and B coefficient, matter-wave interaction: semiclassical treatment, Rabi oscillation, molecular energies and Born-Oppenheimer approximation, types of molecular motion and associated spectroscopy, spectral broadening: homogeneous and inhomogeneous
Unit 2 **(4L)**	**Rotational spectroscopy:** Classical and quantum theory of molecular rotation- rigid rotor, classification of molecular rotors, rotational spectroscopy of diatomic molecules, non-rigid rotor, centrifugal distortion, Stark effect, selection rules, rotational spectra of polyatomic molecules
Unit 3 **(5L)**	**Vibrational spectroscopy:** Review of harmonic oscillator, vibrational selection rules, anharmonic vibrations and Morse oscillator, bond dissociation energies and Birge-Sponer plots, overtones and hot bands, isotopic shift, vibration of polyatomic molecules, normal modes, characteristic group vibrational energies, hydrogen bonds in IR spectra, rotational structure in vibrational spectra of diatomic molecules
Unit 4 **(4L)**	**Raman Spectroscopy**: Description of Raman scattering, Rayleigh scattering, Stokes and anti-Stokes shift, polarizability of the molecules, Placzek theory, selection rules for rotational Raman spectra of diatomic molecules, rotational, vibrational and ro-vibrational Raman spectra, Raman spectra of polyatomic molecules

Unit 5 **(4L)**	**Electronic Spectroscopy:** Born-Oppenheimer approximation, electronic transition, energy of electronic transition, selection rules, Franck-Condon principle, term symbols for atomic and molecular states, Russel-Saunders coupling, selection rules, absorption intensity, probability of light absorption, classification of electronic transition, d-d and CT transitions
Unit 6 **(4L)**	**Emission Spectroscopy:** Fluorescence and phosphorescence, Jablonski diagram, deactivation processes, internal conversion, non-radiative and radiative transitions, characteristic of fluorescence emission, Stokes shift, fluorophores, quantum yield of a fluorescent process, phosphorescence, intersystem crossing, Kasha's rule of the quantum yield of luminescence
Unit 7 **(2L)**	**Photoelectron spectroscopy:** Photoelectric effect, UV photoelectron spectroscopy, X-ray photoelectron spectroscopy, electron binding energy, ESCA, Auger electron spectroscopy
Unit 8 **(4L)**	**NMR Spectroscopy:** Nuclear spin angular momentum, the magnetic moment of a nucleus, the nuclei in a magnetic field, Larmor frequency, chemical shift, electronic shielding of nuclei, scale, pulse sequence, spin-spin and spin lattice relaxation, molecular structure from NMR spectra
Unit 9 **(3L)**	**EPR Spectroscopy:** Stern-Gerlach experiment, electron spin, paramagnetic species, magnetic properties of the electron and selected particles, magnetogyric ratio, electron spin–orbit couplings, energy levels and allowed EPR transitions

TEXT BOOKS/ REFERENCE BOOKS: -

1. C. N. Banwell & E. M. McCash, Fundamentals of Molecular Spectroscopy, McGraw Hill, 2017
2. P. Bernath, Spectra of Atoms and Molecules, OUP, 1995
3. J. M. Hollas, Modern Spectroscopy, Wiley, 2004.
4. P. R. Bunker & P. Jensen, Molecular Symmetry and Spectroscopy, NRC, 2006
5. J. K. M. Sanders & B. K. Hunter, Modern NMR Spectroscopy, OUP, 1993

Jyoti Joshi

Lecture Plan

Lecture No.	Topics to be covered
1	Classical and quantum theory of light
2	absorption and emission of radiation by molecular species, Einstein A and B coefficient
3	matter-wave interaction: semiclassical treatment, Rabi oscillation
4	molecular energies and Born-Oppenheimer approximation
5	types of molecular motion and associated spectroscopy
6	spectral broadening: homogeneous and inhomogeneous
7	Classical and quantum theory of molecular rotation- rigid rotor
8	classification of molecular rotors, rotational spectroscopy of diatomic molecules
9	non-rigid rotor, centrifugal distortion
10	Stark effect, selection rules, rotational spectra of polyatomic molecules
11	Review of harmonic oscillator, vibrational selection rules
12	anharmonic vibrations and Morse oscillator, bond dissociation energies and Birge-Sponer plots, overtones and hot bands, isotopic shift
13	vibration of polyatomic molecules, normal modes
14	characteristic group vibrational energies, hydrogen bonds in IR spectra
15	rotational structure in vibrational spectra of diatomic molecules
16	Description of Raman scattering, Rayleigh scattering, Stokes and anti-Stokes shift
17	polarizability of the molecules, Placzek theory
18	selection rules for rotational Raman spectra of diatomic molecules, rotational, vibrational and ro-vibrational Raman spectra
19	Raman spectra of polyatomic molecules
20	Born-Oppenheimer approximation,
21	electronic transition, energy of electronic transition
22	Franck-Condon principle, term symbols for atomic and molecular states, Russel-Saunders coupling, selection rules

23	absorption intensity, probability of light absorption, classification of electronic transition, d-d and CT transitions
24	Fluorescence and phosphorescence, Jablonski diagram
25	deactivation processes, internal conversion, non-radiative and radiative transitions
26	characteristic of fluorescence emission, Stokes shift, fluorophores, quantum yield of a fluorescent process
27	phosphorescence, intersystem crossing, Kasha's rule of the quantum yield of luminescence
28	Photoelectric effect, UV photoelectron spectroscopy,
29	X-ray photoelectron spectroscopy, electron binding energy, ESCA, Auger electron spectroscopy
30	Nuclear spin angular momentum, the magnetic moment of a nucleus, ,
31	the nuclei in a magnetic field, Larmor frequency, chemical shift
32	electronic shielding of nuclei, scale, pulse sequence, spin-spin and spin lattice relaxation
33	molecular structure from NMR spectra
34	Stern-Gerlach experiment, electron spin, paramagnetic species
35	magnetic properties of the electron and selected particles, magnetogyric ratio, electron spin–orbit couplings
36	energy levels and allowed EPR transitions

DETAILS OF THE COURSE

Course Type	Course Code	Course Title	Credits	Lecture	Tutorial	Practical	Studio
PC	24CYTXX X	Concepts in chemical kinetics and dynamics	3	3	0	0	0

PREREQUISITE

Basic understanding of Quantum Mechanics, and Statistical mechanics

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COURSE OBJECTIVE(s): There are some basic concepts which all physical chemists use to describe chemical reactions. This course five a detailed mathematical introduction of all key concepts with various applications in chemistry.

COURSE OUTCOMES:

CO1	Student learn all key concepts requied in the description of chemical dynamics.
CO2	This course will prepare students will learn the mathematical description for all the chemical dynamic concepts.

COURSE ASSESSMENT

The Course Assessment (culminating to the final grade) will be made up of the following three components;

S. No.	Component	Weightage
1.	Internal assessment (based upon assignments, quizzes and attendance)	20%
2.	Mid-term examination	30%
3.	End Semester Examination	50%

COURSE CONTENTS

Course Content	
Module 1 (6 L)	**Chemical Equilibrium:** Legendre Transformation, Gibbs Free Energy and other thermodynamic potentials,activity coefficients
Module 2 (8 L)	**Activation Energy:** Temperature dependence of rate constants, Arrhenius equation, Tolman Interpretation, Negative activation energy, Modern Interpretation of Activation energy
Module 3 (6 L)	**Potential Energy Surface:** Born-Oppenheimer Approximation, Adiabatic and Diabatic representation, Non-Adiabatic coupling
Module 4 (6 L)	**Reaction Coordinate**: Generalized coordinate, Lagrangian and Hamiltonian mechanics, Minimum Energy Path, Reaction path Hamiltonian, Path Curvature

Module 5 (8 L)	**Reaction Rate Theory:** Concept of Flux, Statistical rate theories Rate from correlation functions
Module 6 (6 L)	**Tunneling in Chemistry:** Simple 1-D models (Echart, Wigner, Bell, WKB approximation) , Small curvature tunneling, Large Curvature Tunneling

Module 7 (6 L)	**Reaction in Solution Phase:** Kramers Theory, Marcus Theory
Reference	R1: Keith J. Laidler Chemical Kinetics R2: Paul L. Houston Chemical Kinetics and Reaction Dynamics R3: J. I. Steinfeld, J. S. Francisco, W. L. Hase Chemical kinetics and dynamics R4: Statistical Mechanics: Donals A Mcquarrie R5:George C. Schatz, Mark A. ratner Quantum Mechanics in Chemistry R6: David Tannor, Introduction to Quantum Mechanics: A time-dependent perspective R7: Herbert Goldstein Classical Mechanics

Lecture Plan

Sl. No.	Lectures	Topic	Text book/ Reference book
		Module-I Chemical Equilibrium :	
		Total Lectures: 5	
	L1-L2	Thermodynamic potentials	R1, R2,R3,R4
-	L3	Legendre Transformation	R1, R2,R3,R4
	L4	Equilibrium Constant in terms of partition function	R1, R2,R3,R4
	L5	Thermodynamic Tables	R4
		Assignment 1 ,	
		Module- II Activation Energy:	

		Total Lectures : 06	
-	L6-L7	Temperature dependence of rate constants, Arrhenius equation	R1, R2
-	L8	Negative activation energy,	R1, R2
	L09-L11	Tolman Interpretation, Modern Interpretation of Activation energy	R1, R2,R3
		Assignment 2	
		Module- III Potential Energy Surface:	
		Total Lectures: 9	
	L12-L14	Born-Oppenheimer Approximation, Electronic structure methods	R1, R2, R3, R5
-	L15-L16	Adiabatic and Diabatic representation	R1, R2, R3, R5
	L17-L18	Non-Adiabatic coupling	R1, R2, R3, R5
	L19-L20	Potential Energy fitting, Neural network	
		Assignment 3	
		Module- IV Reaction Coordinate:	
		Total Lectures: 7	
	L21-L22	Generalized coordinate, Lagrangian and Hamiltonian mechanics	R7
	L23-L24	Minimum Energy Path	R1, R2, R3, R5
	L25	Reaction path Hamiltonian	R1, R2, R3, R5
	L26-L27	Path Curvature	R1, R2, R3, R5
		Module- V Reaction Rate Theory:,	
		Total Lectures: 85	
	L28	Concept of Flux	R5,R6,R7
	L29-L31	Statistical rate theories	R5, R6, R7
	L32	Rate from correlation functions	R1, R2, R3, R5

		Module- VI Tunneling in Chemistry:	
		Total Lectures: 4	
	L33-L34	*Simple 1-D models (Echart, Wigner, Bell, WKB approximation)*	R5,R6,R7
	L35	*Small curvature tunneling, Large Curvature Tunneling*	R5, R6, R7
	L36	Instanton Theories	R5,R6,R7
		Module- VI Reaction in Solution Phase:,	
		Total Lectures: 4	
	L37-L38	Kramers Theory	R5,R6,R7
	L39-L40	Marcus Theory	R5, R6, R7

DETAILS OF THE COURSE

Course Type	Course Code	Course Title	Credits	Lecture	Tutorial	Practical	Studio
PC	24CYTXX X	Environmental Chemistry	3	3	0	0	0

PREREQUISITE

None

COURSE OBJECTIVE(s)

Students will acquire knowledge of importance of environmental chemistry, an interdisciplinary science that involve physics, chemistry, life science and agriculture. They will understand importance of protection and conservation of our environment and need to restrain anthropogenic activities responsible for extensive release of pollutants in environment.

COURSE OUTCOMES:

CO 1	Students will be able to understand that environmental chemistry is a part of environmental educations
CO 2	They will get the knowledge of chemistry involved in atmosphere, air pollution, and water pollution
CO 3	Information about the various environmental episodes

COURSE ASSESSMENT

The Course Assessment (culminating to the final grade) will be made up of the following three components;

S. No.	Component	Weightage
1.	Internal assessment (based upon assignments, quizzes and attendance)	20%
2.	Mid-term examination	30%
3.	End Semester Examination	50%

COURSE CONTENTS

(No. of lectures- 36)

Course Content	
Module1 (4L)	Introduction: concept and scope of environmental chemistry. Environmental segments, Natural and Man-made Disasters, green chemistry
Module 2 (8L)	Atmosphere: Composition of Atmosphere, temperature profile, Properties of troposphere, Temperature inversion. Particles, ions and radicals in atmosphere, chemical and photochemical reactions in atmosphere, Ozone formation with mechanisms, catalytic Ozone depletion, Control Strategies.
Unit 3 (10L)	Water Pollution Introduction of Water pollutants, classification of pollutants like dyes, Pesticides, phenols, toxic metals, chemical speciation (copper, Lead, Mercury, Arsenic, Selenium, Chromium), water quality parameters and standards, Acid rain with chemical reactions, Monitoring techniques and methodology, Fluorosis, Eutrophication
Unit 4 (10L)	Air Pollution: Air pollutants and their classifications. Carbon mono-oxides, Nitrogen oxides, Hydrocarbons and photochemical smog, Aerosols-sources, size distribution and effect on visibility, climate and health. Sources of greenhouse gases, Global warming potentials. Climate change and consequences. Oxidation reactions. Damaging effects on aquatic life, plants, buildings and health. Monitoring of SO2 and NOx. Acid rain control strategies.
Unit 5 (4L)	Chemical toxicology:

Jyoti Joshi

	Toxic chemicals in the environment, Impact of toxic chemicals on enzymes, biochemical effects, Ozone and PAN, Cyanides,and pesticides; Carcinogens, Bio-warfare Agents, Environment and public health

TEXT BOOKS/ REFERENCE BOOKS: -

1. Colin Baird, W.H. Freeman, Environmental Chemistry, Co. New York, 1998.
2. R.P. Wayne, Chemistry of Atmospheres, Oxford Publishers, 2022.
3. A.K. De, Environment Chemistry, Wiley Eastern, 2024.
4. S.E. Manahan, Environmental Chemistry, Lewis Publishers, 2006

Lecture Plan

Lecture No.	Topics to be covered
1	**Unit-I:** Introduction: Concept and scope of environmental chemistry.
2	Discussions on Environmental segments,
3	Natural and Man-made Disasters,
4	Introduction to Green chemistry, Principals and implementations
5	**Unit- II Atmosphere:** Composition of Atmosphere
6	Temperature profile of various segments
7	Properties of troposphere, Temperature inversion.
8	Particles, ions and radicals in atmosphere,
9	chemical and photochemical reactions in atmosphere,
10	Ozone formation with mechanisms
11	Catalytic Ozone depletion,
12	Recent updates and control Strategies
13	**Unit-III Water Pollution** Introduction of Water pollutants,
14	Classification of pollutants like dyes, Pesticides, phenols, toxic metals and other related species
15	Chemical speciation of copper, Lead,
16	Chemical speciation of Mercury, Arsenic,
17	Chemical speciation of Selenium, Chromium

18	water quality parameters and standards,
19	Acid rain with chemical reactions
20	Monitoring techniques and methodology,
21	Fluorosis, Eutrophication
22	Remediation strategies of water pollutants -I
23	Remediation strategies of water pollutants -II
24	**Unit-IV: Air Pollution:** Air pollutants and their classifications
25	Carbon mono-oxides, Nitrogen oxides,
26	Hydrocarbons and photochemical smog,
27	Aerosols-sources, size distribution and effect on visibility
28	climate and health, Sources of greenhouse gases,
29	Global warming potentials. Climate change and consequences
30	Oxidation reactions. Damaging effects on aquatic life, plants, buildings and health
31	Monitoring of SO2 and NOx
32	Acid rain control strategies-I
33	**Unit-V Chemical toxicology:** Toxic chemicals in the environment, Carcinogens,
34	Impact of toxic chemicals on enzymes, biochemical effects,
35	Ozone and PAN, Cyanides,and pesticides;
36	Bio-warfare Agents, Environment and public

DETAILS OF THE COURSE

Course Type	Course Code	Course Title	Credits	Lecture	Tutorial	Practical	Studio
PC	24CYTXXX	Introduction to Density Functional theory	3	3	0	0	0

PREREQUISITE : Basic understanding of Quantum Chemistry

COURSE OBJECTIVE(s): Density-functional theory (DFT) is a modern computational quantum mechanical modelling method which is used in almost every branch of sciences and engineering. In this course student will learn basic principles of DFT with emphasis on in hand experience of DFT calculations.

COURSE OUTCOMES:

CO1	It will give a broad idea about how a multi-electron electronic structure problem can be solved.
CO2	This course will also give some in hand experience for performing DFT calculations along with introduction of many modern DFT functional.

COURSE ASSESSMENT

The Course Assessment (culminating to the final grade) will be made up of the following three components;

S. No.	Component	Weightage
1.	Internal assessment (based upon assignments, quizzes and attendance)	20%
2.	Mid-term examination	30%
3.	End Semester Examination	50%

Course Content	
Module1 (4L)	**Review of Quantum Mechanics:** Time independent Schrodinger Equation, Eigen value problem, exactly solvable one electron systems.
Module 2 (14L)	**Many electron problem:** Pauli antisymmetry principle, Slater determinant, Hartree-Fock Theory, Configuration Interaction, Coupled Cluster theory.

Module 3 (14L)	**Density based approach:** Thomas-Fermi model, Hohenberg-Kohn theorems, Kohn-Sham equations, Exchange and correlation functionals, Local density approximation, Generalized gradient approximation, Adiabatic connection, Hybrids functionals.
Module4 (4L)	Popular Functionals: B3LYP, PBE, B3LYP-D, Minnesota Functionlas etc.
Module 5 (3L)	**Solid state calculations:** Bloch Theorem, Periodic boundary condition , Fourier Transformation, Band calculation.
Reference s	R1: Koch and Max C. Holthausen; A Chemist's Guide to Density Functional Theory (Wiley) R2: Robert Parr ; Density-functional theory of atoms and molecules (OUP USA) R3: David S. Sholl and J. A. Steckel ; Density Functional Theory: A Practical Introduction (Wiley-Interscience) R4: C. Fiolhais, F. Nogueira, Miguel A.L. Marques; A Primer in Density Functional Theory (Springer) R5: A. Szabo and N. S. Ostlund; Modern quantum chemistry (Dover Publications)

Lecture Plan

Sl. No.	Lectures	Topic	Text book/ Reference book
		Module-I Review of Quantum Mechanics:	
		Total Lectures: 4	
	L1	Time independent Schrodinger Equation	R5
-	L2	Eigen value problem	R5

	L3-L4	Exactly solvable one electron systems	R5
		Assignment 1	
		Module- II Many electron problem:	
		Total Lectures : 14	
-	L5-L6	Pauli antisymmetry principle, Slater determinant	R5
	L7-L08	Basis Sets	
-	L9-L10	Hartree-Fock Theory	R5
	L11-L14	Configuration Interaction	R5
	L15-L18	Coupled Cluster theory	R5
		Assignment 2	
		Module- III Density based approach:	
		Total Lectures: 14 **Total Tutorials:**	
	L19	Thomas-Fermi model	R1, R2, R3,R4
-	L20-L25	Hohenberg-Kohn theorems, Kohn-Sham equations, Exchange and correlation functionals	R1, R2, R3,R4
	L26-L30	Local density approximation, Generalized gradient approximation	R1, R2, R3,R4
-	L31-L34	Adiabatic connection, Hybrids functionals	R1, R2, R3,R4
		Assignment 3	
		Module- IV Popular Functionals:	
		Total Lectures: 3	
	L35-L37	B3LYP, PBE, B3LYP-D, Minnesota Functionlas	R1, R2, R3,R4

		Assignment 3	

Jyoti Joshi

		Module- VI: Solid state calculations:	
		Total Lectures: 4	
	L38	Bloch Theorem, Periodic boundary condition	R1, R2, R3,R4
	L39	Fourier Transformation	R1, R2, R3,R4
	L40-L41	Band calculation	R1, R2, R3,R4

DETAILS OF THE COURSE

Course Type	Course Code	Course Title	Credits	Lecture	Tutorial	Practical	Studio
PC	24CYTXXX	Molecular Spectroscopy	3	3	0	0	0

PREREQUISITE

None

COURSE OBJECTIVE(s)

The course provides an introduction to the knowledge of the underlying theory and methods of various types of spectroscopy encompassing a large window of the electromagnetic spectrum starting from radio wave to X-ray

COURSE OUTCOMES:

CO 1	Understand the nature and underlying physical laws of interaction between molecules and electromagnetic radiation
CO 2	Know the various factors responsible for the spectral shapes we observe
CO 3	Gain fundamental information on how different molecular motions results in different spectroscopic methods
CO 4	Select molecular spectroscopy methods suitable for solving given scientific problem
CO 5	Analyze measured spectra to shed light on the structure, activity of the molecule as well as the environment and physical conditions

Jyoti Joshi

COURSE ASSESSMENT

The Course Assessment (culminating to the final grade) will be made up of the following three components;

S. No.	Component	Weightage
1.	Internal assessment (based upon assignments, quizzes and attendance)	20%
2.	Mid-term examination	30%
3.	End Semester Examination	50%

COURSE CONTENTS

Unit 1 **(6L)**	**1. Matter and radiation:** Classical and quantum theory of light, absorption and emission of radiation by molecular species, Einstein A and B coefficient, matter-wave interaction: semiclassical treatment, Rabi oscillation, molecular energies and Born-Oppenheimer approximation, types of molecular motion and associated spectroscopy, spectral broadening: homogeneous and inhomogeneous
Unit 2 **(4L)**	**Rotational spectroscopy:** Classical and quantum theory of molecular rotation- rigid rotor, classification of molecular rotors, rotational spectroscopy of diatomic molecules, non-rigid rotor, centrifugal distortion, Stark effect, selection rules, rotational spectra of polyatomic molecules
Unit 3 **(5L)**	**Vibrational spectroscopy:** Review of harmonic oscillator, vibrational selection rules, anharmonic vibrations and Morse oscillator, bond dissociation energies and Birge-Sponer plots, overtones and hot bands, isotopic shift, vibration of polyatomic molecules, normal modes, characteristic group vibrational energies, hydrogen bonds in IR spectra, rotational structure in vibrational spectra of diatomic molecules
Unit 4	**Raman Spectroscopy**:

(4L)	Description of Raman scattering, Rayleigh scattering, Stokes and anti-Stokes shift, polarizability of the molecules, Placzek theory, selection rules for rotational Raman spectra of diatomic molecules, rotational, vibrational and ro-vibrational Raman spectra, Raman spectra of polyatomic molecules
Unit 5 (4L)	**Electronic Spectroscopy**: Born-Oppenheimer approximation, electronic transition, energy of electronic transition, selection rules, Franck-Condon principle, term symbols for atomic and molecular states, Russel-Saunders coupling, selection rules, absorption intensity, probability of light absorption, classification of electronic transition, d-d and CT transitions
Unit 6 (4L)	**Emission Spectroscopy**: Fluorescence and phosphorescence, Jablonski diagram, deactivation processes, internal conversion, non-radiative and radiative transitions, characteristic of fluorescence emission, Stokes shift, fluorophores, quantum yield of a fluorescent process, phosphorescence, intersystem crossing, Kasha's rule of the quantum yield of luminescence
Unit 7 (2L)	**Photoelectron spectroscopy:** Photoelectric effect, UV photoelectron spectroscopy, X-ray photoelectron spectroscopy, electron binding energy, ESCA, Auger electron spectroscopy
Unit 8 (4L)	**NMR Spectroscopy:** Nuclear spin angular momentum, the magnetic moment of a nucleus, the nuclei in a magnetic field, Larmor frequency, chemical shift, electronic shielding of nuclei, scale, pulse sequence, spin-spin and spin lattice relaxation, molecular structure from NMR spectra
Unit 9 (3L)	**EPR Spectroscopy**: Stern-Gerlach experiment, electron spin, paramagnetic species, magnetic properties of the electron and selected particles, magnetogyric ratio, electron spin–orbit couplings, energy levels and allowed EPR transitions

TEXT BOOKS/ REFERENCE BOOKS: -

1. C. N. Banwell & E. M. McCash, Fundamentals of Molecular Spectroscopy, McGraw Hill, 2017
2. P. Bernath, Spectra of Atoms and Molecules, OUP, 1995

Jyoti Joshi

3. J. M. Hollas, Modern Spectroscopy, Wiley, 2004.
4. P. R. Bunker & P. Jensen, Molecular Symmetry and Spectroscopy, NRC, 2006
5. J. K. M. Sanders & B. K. Hunter, Modern NMR Spectroscopy, OUP, 1993

Lecture Plan

Lecture No.	Topics to be covered
1	Classical and quantum theory of light
2	absorption and emission of radiation by molecular species, Einstein A and B coefficient
3	matter-wave interaction: semiclassical treatment, Rabi oscillation
4	molecular energies and Born-Oppenheimer approximation
5	types of molecular motion and associated spectroscopy
6	spectral broadening: homogeneous and inhomogeneous
7	Classical and quantum theory of molecular rotation- rigid rotor
8	classification of molecular rotors, rotational spectroscopy of diatomic molecules
9	non-rigid rotor, centrifugal distortion
10	Stark effect, selection rules, rotational spectra of polyatomic molecules
11	Review of harmonic oscillator, vibrational selection rules
12	anharmonic vibrations and Morse oscillator, bond dissociation energies and Birge-Sponer plots, overtones and hot bands, isotopic shift
13	vibration of polyatomic molecules, normal modes
14	characteristic group vibrational energies, hydrogen bonds in IR spectra
15	rotational structure in vibrational spectra of diatomic molecules
16	Description of Raman scattering, Rayleigh scattering, Stokes and anti-Stokes shift
17	polarizability of the molecules, Placzek theory
18	selection rules for rotational Raman spectra of diatomic molecules, rotational, vibrational and ro-vibrational Raman spectra
19	Raman spectra of polyatomic molecules

Jyoti Joshi

20	Born-Oppenheimer approximation,
21	electronic transition, energy of electronic transition
22	Franck-Condon principle, term symbols for atomic and molecular states, Russel-Saunders coupling, selection rules
23	absorption intensity, probability of light absorption, classification of electronic transition, d-d and CT transitions
24	Fluorescence and phosphorescence, Jablonski diagram
25	deactivation processes, internal conversion, non-radiative and radiative transitions
26	characteristic of fluorescence emission, Stokes shift, fluorophores, quantum yield of a fluorescent process
27	phosphorescence, intersystem crossing, Kasha's rule of the quantum yield of luminescence
28	Photoelectric effect, UV photoelectron spectroscopy,
29	X-ray photoelectron spectroscopy, electron binding energy, ESCA, Auger electron spectroscopy
30	Nuclear spin angular momentum, the magnetic moment of a nucleus, ,
31	the nuclei in a magnetic field, Larmor frequency, chemical shift
32	electronic shielding of nuclei, scale, pulse sequence, spin-spin and spin lattice relaxation
33	molecular structure from NMR spectra
34	Stern-Gerlach experiment, electron spin, paramagnetic species
35	magnetic properties of the electron and selected particles, magnetogyric ratio, electron spin–orbit couplings
36	energy levels and allowed EPR transitions

DETAILS OF THE COURSE

Course Type	Course Code	Course Title	Credits	Lecture	Tutorial	Practical	Studio
PC	24CYTXXX	Introduction to Astrochemistry	3	3	0	0	0

PREREQUISITE

High School Chemistry, Physics and Mathematics, Basic quantum mechanics

COURSE OBJECTIVE(s)

The course would cover topics like interstellar medium, atomic and molecular physics, interstellar chemistry, molecular astronomy and unresolved problems.

COURSE OUTCOMES:

CO 1	Gain basic idea about the nature of interstellar medium, classification, physical conditions and their importance in the evolution of universe.
CO 2	Understand the various spectroscopic features important for identifying interstellar molecules and assessing the physical conditions of the medium
CO 3	Understand the different chemical processes, their energetic and kinetic behaviour and importance and utilities of chemical reactions network
CO 4	Learn about various aspects of interstellar molecules, including their energy level structures, their spectra, their chemistry, where they have been detected, and what they tell us as astronomical probes

COURSE ASSESSMENT

The Course Assessment (culminating to the final grade) will be made up of the following three components;

S. No.	Component	Weightage
1.	Internal assessment (based upon assignments, quizzes and attendance)	20%
2.	Mid-term examination	30%
3.	End Semester Examination	50%

COURSE CONTENTS

Unit 1	The Interstellar Medium
(6L)	Introduction to the Interstellar Medium, Conditions, time and length scales, constituents (elemental abundances, isotopic ratios, grains, radiation field, cosmic rays, shocks, magnetic fields). Structure and Evolution of the Interstellar Medium, Three-phase interstellar medium. Heating and cooling. Life cycle of interstellar matter (astration). Types of

Jyoti Joshi

	interstellar environments (diffuse clouds, dense clouds, star forming cores, photodissociation regions).
Unit 2 **(12L)**	**Atomic & Molecular Physics** Interaction of Radiation with Matter: Semi-classical approach, oscillator strengths and Einstein coefficients, introduction to spectroscopy. Atomic structure (principal, angular momentum, magnetic, and spin quantum numbers; fine structure; hyperfine structure), atomic spectroscopy. Structure and Spectra of Diatomic Molecules: Energy level structure (electronic, vibrational and rotational). Electronic, vibrational spectra and rotational spectra. Application to H_2, C_2, CH, CO. Structure and Spectra of Polyatomic Molecules: Energy level structure of spherical, linear, symmetric, and asymmetric tops. Rotation-vibration interaction. Application to H_3^+, C_3, H_2O, HCO^+. Radiative and collisional excitation processes: Radiative excitation and selection rules. Collisional excitation and de-excitation. Rotational excitation of C_2 and CO. Radiative transfer.
Unit 3 **(10L)**	**Interstellar Chemistry** H_2 Formation and Destruction, Formation of H_2 on interstellar grains. Chemical Kinetics and Rate Equations, Ion-Neutral Reaction Dynamics, Types of chemical reactions, endo/exothermicities, activation energies, rate expressions. Langevin cross-sections and temperature independence. Importance of ion-neutral reactions for interstellar chemistry. Chemical Modeling, Calculation of molecular abundances using chemical reaction networks: steady state and time-dependent. Identification of primary formation/destruction pathways for individual molecules. Dependence on laboratory data. Isotopic Fractionation, Quantum mechanical effects leading to fractionation of rare isotopes in molecules, and observational evidence.
Unit 4 **(8L)**	**Molecular Astronomy** Detecting interstellar molecules in the optical spectra, Principles of optical spectrographs, and echelles. Basics of Radioastronomy, Fourier transforms, single dish studies, mapping, backends for spectroscopy, Radio Interferometry, Principles of interferometry (aperture synthesis).

	Interstellar molecules (with special reference to CO, CH^+, HCO^+, H_2CO, NH, N_2H^+, NH_3, OH, H_2O, H_3O^+, C_2H, C_2H_2, C_3H, C_3H_2, CN, HCN, HNC, $HCNH^+$)

(No. of lectures- 10)

TEXT BOOKS/ REFERENCE BOOKS: -

1. A. M. Shaw, Astrochemistry: From astronomy to astrobiology, Wiley, 2006
2. S. Yamamoto, Introduction to Astrochemistry, Springer, 2017
3. D. A. Williams and S. Vitti, Observational Molecular Astronomy, Cambridge University Press, 2013
4. P. Bernath, Spectra of Atoms and Molecules, OUP, 1995
5. K. J. Laidler, Chemical Kinetics, Pearson, 2008
6. Related primary and review articles from literature.

<u>Lecture Plan</u>

Lecture No.	Topics to be covered
1	General Introduction
2	Introduction to the Interstellar Medium (ISM), Conditions, time and length scales
3	Constituents of ISM (elemental abundances, isotopic ratios, grains, radiation field, cosmic rays, shocks, magnetic fields).
4	Structure and Evolution of the Interstellar Medium, Three-phase interstellar medium. Heating and cooling.
5	Life cycle of interstellar matter (astration).
6	Types of interstellar environments (diffuse clouds, dense clouds, star forming cores, photodissociation regions).
7	Interaction of Radiation with Matter: Semi-classical approach, oscillator strengths and Einstein coefficients.
8	Atomic structure (principal, angular momentum, magnetic, and spin quantum numbers; fine structure; hyperfine structure)
9	Introduction to spectroscopy: atomic spectroscopy
10	Structure and Spectra of Diatomic Molecules: Energy level structure (electronic, vibrational and rotational).

11	Electronic, vibrational spectra and rotational spectra.
12	Application to H_2, C_2, CH, CO.
13	Structure and Spectra of Polyatomic Molecules: Energy level structure of spherical, linear, symmetric, and asymmetric tops.
14	Rotation-vibration interaction.
15	Application to H_3^+, C_3, H_2O, HCO^+.
16	Radiative and collisional excitation processes: Radiative excitation and selection rules.
17	Collisional excitation and de-excitation.
18	Rotational excitation of C_2 and CO. Radiative transfer.
19	H_2 Formation and Destruction, Formation of H_2 on interstellar grains.
20	Chemical Kinetics and Rate Equations, Ion-Neutral Reaction Dynamics,
21	Types of chemical reactions, endo/exothermicities, activation energies, rate expressions.
22	Langevin cross-sections and temperature independence.
23	Importance of ion-neutral reactions for interstellar chemistry.
24	Chemical Modeling,
25	Calculation of molecular abundances using chemical reaction networks: steady state and time-dependent.
26	Identification of primary formation/destruction pathways for individual molecules.
27	Dependence on laboratory data. Isotopic Fractionation
28	Quantum mechanical effects leading to fractionation of rare isotopes in molecules, and observational evidence.
29	Detecting interstellar molecules in the optical spectra
30	Principles of optical spectrographs, and echelles.
31	Basics of Radioastronomy, Fourier transforms, single dish studies, mapping, backends for spectroscopy
32	Radio Interferometry, Principles of interferometry (aperture synthesis)
33-36	Interstellar molecules (with special reference to CO, CH^+, HCO^+, H_2CO, NH, N_2H^+, NH_3, OH, H_2O, H_3O^+, C_2H, C_2H_2, C_3H, C_3H_2, CN, HCN, HNC, $HCNH^+$)

DETAILS OF THE COURSE

Course Type	Course Code	Course Title	Credits	Lecture	Tutorial	Practical	Studio
PC	24CYTXXX	Crystallography	3	3	0	0	0

PREREQUISITE

Basic knowledge in Materials Science, Physics, Chemistry, Chemical Engineering, and Nanotechnology.

COURSE OBJECTIVE(s):

The characteristics of crystalline materials depend heavily on their crystal structure and the way atoms are arranged within them. X-ray diffraction is a sophisticated technique used to identify crystal structures and related aspects. This course introduces the basics of X-ray diffraction and explores how it can be applied to address various crystallographic issues in both single and polycrystalline materials.

COURSE OUTCOMES:

CO 1	Grasp the basic principles of structure of materials and crystallography.
CO 2	Understand the physics and application of XRD diffraction
CO 3	Grasp a basic idea to collect, solve and refine the raw single crystal X-ray diffraction data.

COURSE ASSESSMENT

The Course Assessment (culminating to the final grade) will be made up of the following three components;

S. No.	Component	Weightage
1.	Internal assessment (based upon assignments, quizzes and attendance)	20%
2.	Mid-term examination	30%

3.	End Semester Examination	50%

COURSE CONTENTS

Module 1(7 L)	**Introduction** Geometry of Crystals, Reciprocal Lattice; Point Groups and Space Groups, Stereographic Projection, Basics of X-Rays, Production and Detection of X-Rays.
Module 2(10 L)	**Principle** Principles of X-Ray Diffraction, X-Ray Diffraction Methods, Diffractometer Measurements, Intensity of Diffracted Beams, Determination of Crystal structures, Precise Lattice Parameter Determination, Phase Diagram Determination, Ordered Disordered Transformation, Qualitative Phase Analysis, Quantitative Phase Analysis 1.
Module 3 (9 L)	**Data collection** Introduction to diffractometer and collection of SCXRD data. Collection of SCXRD data, Introduction to software related to solve X-ray diffraction (classic to modern) ORTEP; WINGX; PLATON, etc, Software related to solve X-ray diffraction.
Module 4(10 L)	**Solving SCXRD data** Software related to solve X-ray diffraction. Solving Raw data, Software used to read the crystal data like Mercury, Diamond, etc., How to create a CIF files and how to rectify the alerts in the final solved data. and generation of CheckCIF file. Chemical Analysis by X-Ray Fluorescence, Chemical Analysis by X-Ray Absorption., Effect of Crystallite Size on Diffracted X-Ray Intensity.

(No. of lectures- 36)

TEXT BOOKS/ REFERENCE BOOKS: -

[1] William D. Callister, Jr., Materials Science and Engineering: An Introduction, 7th Edition, John Wiley & Sons, (2006). (Chapter 3, 4 & 12).

[2] Maureen M. Julian, Foundations of Crystallography, Taylor & Francis Group (2008).

[3] Martin T. Dove, Structure and Dynamics-An atomic view of materials, Oxford University Press, (2003).

[4] B.D. Cullity and S.R. Stock, Elements of X-ray Diffraction, 3rd edition, Addison-Wesley Publishing Company (2001).

Lecture Plan

Lecture No.	Topics to be covered
1	Geometry of Crystals.
2	Reciprocal Lattice; Point Groups and Space Groups
3	Stereographic Projection
4	Point Groups and Space Groups
5	Point Groups and Space Groups (Cont'd),
6	Basics of X-Rays.
7	Production and Detection of X-Rays.
8	Principles of X-Ray Diffraction.
9	X-Ray Diffraction Methods.
10	Diffractometer Measurements.
11	Intensity of Diffracted Beams.
12	Determination of Crystal structures.
13	Precise Lattice Parameter Determination.
14	Phase Diagram Determination.
15	Ordered Disordered Transformation.
16	Qualitative Phase Analysis.
17	Quantitative Phase Analysis 1.
18	Introduction to diffractometer and collection of SCXRD data.
19	Introduction to diffractometer and collection of SCXRD data (cont.)
20	Collection of SCXRD data
21	Collection of SCXRD data
22	Introduction to software related to solve X-ray diffraction (classic to modern) ORTEP; WINGX; PLATON, etc.
23	ORTEP
24	WINGX
25	PLATON,
26	Software related to solve X-ray diffraction (cont.).
27	Solving Raw data
28	Solving Raw data (cont.)

Jyoti Joshi

29	Solving Raw data (cont.)
30	Solving Raw data (cont.)
31	Software used to read the crystal data like Mercury, Diamond, etc.
32	Software used to read the crystal data like Mercury, Diamond, etc (cont.)
33	How to create a CIF files and how to rectify the alerts in the final solved data. and generation of CheckCIF file.
34	Chemical Analysis by X-Ray Fluorescence, Chemical Analysis by X-Ray Absorption.
35	Effect of Crystallite Size on Diffracted X-Ray Intensity.
36	Effect of Crystallite Size on Diffracted X-Ray Intensity (cont.)

DETAILS OF THE COURSE

Course Type	Course Code	Course Title	Credits	Lecture	Tutorial	Practical	Studio
PC	24CYTX XX	Solid State Chemistry: Fundamentals and Applications	3	3	0	0	0

PREREQUISITE:

Basic understanding of Physical Chemistry

COURSE OBJECTIVE(s):

To identify and apply the concepts involved in the structure, physical properties, syntheses, and characterization of crystalline inorganic solids.

COURSE OUTCOMES:

CO 1	Learning unit cell contents and fractional coordinates, index cubic powder XRD patterns, determine unit cell parameter and lattice types
CO 2	Indexing non-cubic powder XRD patterns based on unit cell parameters provided, and calculating densities from powder XRD data
CO 3	Identifying and applying suitable strategies for synthesizing inorganic crystalline solids in polycrystalline and single crystal forms
CO 4	Correlation and prediction of structure-composition-properties (magnetic, electrical, and optical) in inorganic crystalline solids

COURSE ASSESSMENT

The Course Assessment (culminating to the final grade) will be made up of the following three components:

S. No.	Component	Weightage
1.	Internal assessment (based upon assignments, quizzes and attendance)	20%
2.	Mid-term examination	30%
3.	End Semester Examination	50%

COURSE CONTENTS

Unit I: Crystal Structure: Crystalline (molecular and non-molecular) and amorphous solids, The crystal lattice and unit cells, crystal systems and Bravais lattices, Close packing in solids, Interstitial sites, Structures based on close packing (fcc, bcc and hcp), Layered structures based on close packing, Other important crystal structures (ReO_3, perovskite ABO_3, $YBa_2Cu_3O_7$, spinel, rutile, corundum and olivine), Crystal defects and their classification, Lattice vacancies/interstitials, Intrinsic defects, Extrinsic defects, Defect clusters, Dislocations, Stacking faults, Movement of defects, Grain boundaries, Crystallographic shear. **(No. of lectures: 10)**

Unit II: Preparative Methods of Solids: Substitutional solid solutions, Interstitial/vacancy solid solutions, Cation vacancies, Cation interstitials, Anion vacancies, Anion interstitials, Monitoring of solid solution formation, Fundamentals and mechanistic aspects of solid state reactions, Film deposition, Chemical precursor method, Co-precipitation, Sol-gel, Metathesis, Solution combustion synthesis, Ion exchange reactions, Intercalation/de-intercalation reactions, Hydrothermal, Solvothermal and template synthesis, High pressure synthesis, Mesoscopic assembly, Microwave and sonochemistry approach for the synthesis of solids, Solution growth, Hydrothermal method, Chemical vapor transport, Melt growth - Bridgeman, Czochralski, Kyropoulus, Verneuil, Epitaxial growth of thin films, Fused salt electrolysis; Flux growth.

(No. of lectures: 10)

UNIT III: Characterization of Solids by Physical Techniques: Powder X-ray diffraction (PXRD) – Indexing the PXRD patterns, Structure factor, Determination of lattice type, Unit cell parameter and density from the PXRD patterns, High temperature PXRD, Electron and neutron diffraction, microscopic techniques – Optical and electron microscopy, Spectroscopic techniques – XRF, ESCA, XPS, UPS, EELS, TGA, DTA and DSC, Applications – Glasses, Polymorphic phase transition, Decomposition pathway determination, Enthalpy and heat capacity measurements. **(No. of lectures: 10)**

UNIT IV: Electronic and Electrical Properties of Solids: Band theory to determine electronic structure of solids, Band structures of metals, semiconductors and insulators, Controlled vacancy semiconductors, Thermoelectric effects - Thomson, Peltier and Seebeck, Hall effect, Thermocouples, Dielectric materials, Ferroelectricity, Pyroelectricity, Piezoelectricity and Multiferroics. **(No. of lectures: 6)**

TEXT BOOKS/ REFERENCE BOOKS:

1. A. R. West, Solid State Chemistry and its Applications, John Wiley & Sons, 2007.
2. L. E. Smart and E. A. Moore, Solid State Chemistry - An Introduction, 4th Edition, CRC Press, 2012.
3. H. V. Keer, Principles of the Solid State, 2nd Edition, New Age International, 2017.
4. David Segal, Chemical Synthesis of Advanced Ceramic Materials, Cambridge University Press, 1989.
5. Richard Tilley, Crystals and Crystal Structures, John Wiley & Sons, 2006.

Lecture Plan

Lecture No.	Topics to be covered
1	Crystalline (molecular and non-molecular) and amorphous solids, The crystal lattice and unit cells
2	Crystal systems and Bravais lattices, Close packing in solids
3	Interstitial sites, Structures based on close packing (fcc, bcc and hcp)
4	Layered structures based on close packing
5	Other important crystal structures (ReO_3, perovskite ABO_3, $YBa_2Cu_3O_7$, spinel, rutile, corundum, and olivine)
6	Crystal defects and their classification
7	Lattice vacancies/interstitials, Intrinsic defects
8	Extrinsic defects, Defect clusters
9	Dislocations, Stacking faults, Movement of defects
10	Grain boundaries, Crystallographic shear
11	Substitutional solid solutions, Interstitial/vacancy solid solutions
12	Cation vacancies, Cation interstitials, Anion vacancies, Anion interstitials
13	Monitoring of solid solution formation, Fundamentals, and mechanistic aspects of solid-state reactions
14	Film deposition, Chemical precursor method, Co-precipitation
15	Sol-gel, Metathesis, Solution combustion synthesis
16	Ion exchange reactions, Intercalation/de-intercalation reactions, Hydrothermal, Solvothermal and template synthesis
17	High pressure synthesis, Mesoscopic assembly, Microwave and sonochemistry approach for the synthesis of solids
18	Solution growth, Hydrothermal method
19	Chemical vapor transport, Melt growth - Bridgeman, Czochralski, Kyropoulus, Verneuil, Epitaxial growth of thin films
20	Fused salt electrolysis; Flux growth method

21	Powder X-ray diffraction (PXRD) – Indexing the PXRD patterns
22	Structure factor, Determination of lattice type
23	Unit cell parameter and density from the PXRD patterns
24	High temperature PXRD, Electron and neutron diffraction
25	Microscopic techniques – Optical and electron microscopy
26	Spectroscopic techniques – XRF, ESCA, XPS, UPS
27	EELS, TGA, DTA and DSC
28	Glasses, Polymorphic phase transition
29	Decomposition pathway determination
30	Enthalpy and heat capacity measurements.
31	Band theory to determine electronic structure of solids
32	Band structures of metals, semiconductors, and insulators
33	Controlled vacancy semiconductors
34	Thermoelectric effects - Thomson, Peltier and Seebeck, Hall effect,
35	Thermocouples, Dielectric materials
36	Ferroelectricity, Pyroelectricity, Piezoelectricity and Multiferroics.

DETAILS OF THE COURSE

Course Type	Course Code	Course Title	Credits	Lecture	Tutorial	Practical	Studio
PC	24CYTXXX	Laser Spectroscopy: Theory and Applications	3	3	0	0	0

PREREQUISITE

Basic Mathematics, Quantum Mechanics and Spectroscopy

COURSE OBJECTIVE(s)

The course would impart fundamental and application based knowledge to understanding the construction and function of laser and its various uses in spectroscopic methods used in physics, chemistry and biology.

COURSE OUTCOMES:

CO 1	The course provides an overview of the fundamental concepts of laser operation.
CO 2	It enables the students to compare the function, properties and application of various types of common lasers.
CO 3	It gives a detailed idea of a number of fundamental as well as advanced laser based spectroscopic methods and their applications in studying photochemical and photophysical processes important from chemical and biological perspectives.

COURSE ASSESSMENT

The Course Assessment (culminating to the final grade) will be made up of the following three components;

S. No.	Component	Weightage
1.	Internal assessment (based upon assignments, quizzes and attendance)	20%
2.	Mid-term examination	30%
3.	End Semester Examination	50%

COURSE CONTENTS

Module 1 (7 L)	**Light Matter Interaction** Absorption, emission and scattering, Einstein A & B coefficient, polarizability model, light-matter interaction: semiclassical treatment, Rabi oscillation, linewidth, homogeneous and inhomogeneous line broadening.
Module 2 (7 L)	**Laser Operation** Population inversion: 3 & 4 level system, gain and threshold, resonator

Jyoti Joshi

	cavity, optical pumping, CW lasers, Q-switching and mode locking: pulsed lasers. Different types of lasers: atomic lasers (He-Ne), gas lasers (CO_2 and N_2), excimer lasers, solid state lasers (Nd:YAG, Ti:Saphire).
Module 3 (5L)	**Spectroscopy in Molecular Beam** Cavity ring-down spectroscopy, laser induced fluorescence, double resonance spectroscopy (UV-UV and IR-UV), resonance enhanced two-photon and multi photon ionisation spectroscopy (R2PI and REMPI) and their applications.
Module 4 (10 L)	**Laser Raman Spectroscopy** Resonance Raman spectroscopy, stimulated Raman spectroscopy, surface enhanced Raman spectroscopy (SERS), coherent anti-Stokes Raman spectroscopy (CARS) and their applications.
Module 5 (7 L)	**Ultrafast Spectroscopy** Pump-probe spectroscopy, transient absorption spectroscopy, fluorescence up-conversion spectroscopy, 2D IR spectroscopy and their applications.

TEXT BOOKS/ REFERENCE BOOKS: -

1. W. Demtröder, Laser Spectroscopy Vol. 1: Basic Concepts and Instrumentation, Springer, 2002
2. W. T. Silfvast, Laser Fundamentals, Cambridge University Press, 2016.
3. J. M. Hollas, High Resolution Spectroscopy, Wiley, 1998.
4. H. H. Telle, A. G. Urena, R. J. Donovan, Laser Chemistry: Spectroscopy, Dynamics and Applications, Wiley, 2007.
5. W. Demtröder, M. Inguscio, Applied Laser Spectroscopy, Plenum Press, 1990.

Lecture Plan

Lecture No.	Topics to be covered
1	What is Absorption, Its principle and applications.
2	Emission and scattering,
3	Einstein A & B coefficient,
4	Polarizability model,

5	Light-matter interaction: semiclassical treatment,
6	Rabi oscillation, linewidth.
7	Homogeneous and inhomogeneous line broadening
8	Population inversion: 3 & 4 level system,
9	Gain and threshold, resonator cavity,
10	Optical pumping, CW lasers, Q-switching and mode locking: pulsed lasers.
11	Different types of lasers: atomic lasers (He-Ne).
12	Gas lasers (CO_2 and N_2).
13	Excimer lasers,
14	Solid state lasers (Nd:YAG, Ti:Saphire).
15	Cavity ring-down spectroscopy,
16	Laser induced fluorescence,
17	Double resonance spectroscopy (UV-UV and IR-UV),
18	Resonance enhanced two- photon and
19	Multi-photon ionisation spectroscopy (R2PI and REMPI) and their applications.
20	Resonance Raman spectroscopy,
21	Stimulated Raman spectroscopy,
22	Stimulated Raman spectroscopy(cont.)
23	Stimulated Raman spectroscopy, (cont.)
24	Surface enhanced Raman spectroscopy (SERS) (cont.)
25	Surface enhanced Raman spectroscopy (SERS) (cont.)
26-29	Coherent anti-Stokes Raman spectroscopy (CARS) and their applications.
30	Pump-probe spectroscopy,
31	Transient absorption spectroscopy,
32	Fluorescence up-conversion spectroscopy,
33	Fluorescence up-conversion spectroscopy. (cont.)

Jyoti Joshi

34	2D IR spectroscopy
35	2D IR spectroscopy (cont.)
36	2D IR spectroscopy applications