SRI SATHYA SAI INSTITUTE OF HIGHER LEARNING

(Deemed to be University)

Syllabus for
M.Sc. in Chemistry

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Sri Sathya Sai District, A.P. - 515 134
India

17-10-2022

SRI SATHYA SAI INSTITUTE OF HIGHER LEARNING
(Deemed to be University)

Department of Chemistry

Syllabus for Two Year M.Sc. in Chemistry

The Masters course in Chemistry will consist of eighteen theory papers (including Mathematics for Chemistry), eight practical papers and a project spread over two semesters. During this period all aspects of the different branches of Chemistry will be covered in a manner so that the students get as complete a picture as possible of the range and depth of the subject. The emphasis is on detailed understanding of the fundamental principles and giving training in appropriate computational and experimental methods. The objective is to provide rigorous training in all the major branches of Chemistry. In the final semester, advanced topics in emerging fields are introduced to enable the students to have a good knowledge of current trends in research across the domains of Chemistry. Electives in frontier and interdisciplinary areas are also offered in the fourth semester. A special elective paper in the field of Bio-catalysis is included so as to give the students an in-depth expertise in the use of green chemistry for technology. A student graduating with an M.Sc. degree in Chemistry will have gained exposure to almost every aspect of the field – Theoretical, Applied, Instrumental, Computational and Experimental Chemistry.

Vision

To positively enrich exploration and excellence in new chemical frontiers through socially relevant research, innovations and collaborations.

Mission

In-depth understanding and Training

- रसोवैसः (RasoVaiSah):Educate about how Chemistry is the essence of all living systems and physical processes

- Teach basic concepts along with advances in the subject
- Synergy between theory and experiments
- Training in relevant computational and experimental methods
- Ignite the passion towards scientific endeavors and train students into research-oriented scientists with noble ambitions

Inspiring design and innovation

- Establish a learning program that aids innovation
- Design and model molecules that mimic biomolecules in nature.
- Inspire research with social relevance.

Create and Collaborate

- Design novel materials for energy storage, drug delivery, bio-imaging, water purification and sensing applications
- Remove barriers between conventional branches of Chemistry and explore collaboration within and outside SSSIHL

Values

- Mentoring students to inculcate the philosophy that "Education is for life and not for living"
- Value-oriented teaching of subjects in innovative ways that blend human values with knowledge. This is a constant endeavor.

Program Specific Outcomes(PSOs)

The Master's program offered by the Department of Chemistry equips the students with in-depth understanding of the fundamentals in all the major domains of Chemistry. It aims to provide the graduate with a right mix of theory, application, instrumentation, computational and experimental skills in Chemistry in tune with the latest advancements in the field. The acquired skills,

knowledge and kindled spirit of research inspire the student to explore the vast world of Chemistry.
The Department brings together all the major branches of Chemistry with appropriate computational and experimental methods. The program is designed to explore and promote translational research on environment, health and energy with specific focus on thrust areas dealing with sensing technology, bioprocessing, bioremediation,synthesis/semi-synthesis of biologically active compounds, nanotechnology and plasmonics. The objective of the program is to develop a good command over the subject with which the student can ably perform in industry and/or in academics.

The program provides advanced courses in Quantum Chemistry and Group Theory, Analytical Chemistry, Chemical Kinetics, Surface Chemistry, Polymer Chemistry, Statistical Thermodynamics, Electrochemistry, Spectroscopy, Environmental Chemistry, Medicinal Chemistry and Synthetic Organic Chemistry. In addition to these, the courses in emerging fields like Functional Materials, Bio-catalysis, Supramolecular Chemistry, Computational Applications in Chemistry coupled with the hands-on experience gained from relevant project work, equips the post-graduate with all the basic skills and experience to identify their area of interest and pursue higher studies through research or through a job in industry/academia.

Attainment of POs and PSOs

We keep a tab on the alumni placement and their performances across the world to informally evaluate the success of our program outcomes. The rigorous internal assessment constitutes *viva-voce* and continuous internal evaluation. The end-semester examinations instituted by the University includes internal/external question paper setting along with double evaluation. Timely continuous look at the overall performance of the students leads to appropriate measures.

DEPARTMENT OF CHEMISTRY
SCHEME OF INSTRUCTION AND EVALUATION
M.Sc. (CHEMISTRY)
(Effective 2022/23 batch onwards)

Paper Code	Title of the Paper	Credits	Hours	Mode of Evaluation	Type of Papers	Maximum Marks
Semester I						
PCHM-101(i)	Quantum Chemistry and Group Theory	3	3	IE2	T	100
PCHM-101(ii)	Mathematics for Chemistry	Non-Credit	2	-	T	--
PCHM-102	Analytical Chemistry	3	3	IE2	T	100
PCHM-103	Coordination Chemistry	3	3	IE2	T	100
PCHM-104	Advanced Aspects of Organic Structure and Stereochemistry	3	3	IE2	T	100
PCHM-105	Practical: Coordination Chemistry (Preparation and Analysis)	2	6	I	P	50
PCHM-106	Practical: Analytical Chemistry	2	6	I	P	50
PCHM-107	Practical: Organic Qualitative Analysis (Mixture Separation and Analysis and Drug Analysis)	2	6	I	P	50
PAWR-100	Awareness Course – I: Education for Life	1	2	I	T	50
		19 credits	34 Hours			600 marks

Paper Code	Title of the Paper	Credits	Hours	Mode of Evaluation	Type of Papers	Maximum Marks
Semester II						
PCHM-201	Structural Inorganic and Bio-Inorganic Chemistry	3	3	IE2	T	100
PCHM-202	Chemical Kinetics and Surface Chemistry	3	3	IE2	T	100
PCHM-203	Statistical Thermodynamics and Electrochemistry	3	3	IE2	T	100
PCHM-204	Physical and Mechanistic Aspects of Organic Chemistry	3	3	IE2	T	100

PCHM-205	Practical: Inorganic Chemistry	2	6	I	P	50
PCHM-206	Practical: Physical Chemistry	2	6	I	P	50
PCHM-207	Practical: Organic Synthesis (multistep) and Spectral Analysis	2	6	I	P	50
PAWR-200	Awareness Course – II: God, Society and Man	1	2	I	T	50
		19 credits	32 hours			600 marks

Semester III						
PCHM-301	Organometallic Chemistry	3	3	IE2	T	100
PCHM-302	Polymer Chemistry and Applications of Group Theory	3	3	IE2	T	100
PCHM-303	Synthetic Organic Chemistry	3	3	IE2*	T	100
PCHM-304	Theory and Application of Physical Methods in Chemistry	3	3	IE2*	T	100
PCHM-305	Practical: Computational Applications in Chemistry-I	2	6	I	P	50
PCHM-306	Project work (Interim Review) **	-	12	I	PW	50**
PAWR-300	Awareness Course –III: Guidelines for Morality	1	2	I	T	50
		15 credits	32 hours			550 marks

Semester IV						
PCHM-401	Solid State Chemistry and Nano Materials	2	2	IE2	T	50
PCHM-402	Supramolecular Chemistry	2	2	IE2	T	50
PCHM-403	Medicinal Chemistry	2	2	IE2	T	50
PCHM-404	Elective–I	3	3	IE2*	T	100
PCHM-405	Elective–II	3	3	IE2*	T	100

PCHM-406	Practical: Computational Applications in Chemistry-II	2	6	I	P	50
PCHM-407	Project Work ***	8***	12	E	PW	200***
PAWR-400	Awareness Course –IV: Wisdom for Life	1	2	I	T	50
		23 credits	**32** Hours			**650** marks
	GRAND TOTAL	**76** credits	**132** Hours			**2400** marks

Modes of Evaluation	Types of Papers

Modes of Evaluation

Indicator	Legend
IE1	CIE and ESE; ESE single evaluation
IE2	CIE and ESE; ESE double evaluation
I	Continuous Internal Evaluation (CIE) only Note: 'I' does not connote 'Internal Examiner'
E	End Semester Examination (ESE) only Note: 'E' does not connote 'External Examiner'
E1	ESE single evaluation
E2	ESE double evaluation

Continuous Internal Evaluation (CIE) & End Semester Examination (ESE)

Types of Papers

Indicator	Legend
T	Theory
P	Practical
V	*Viva voce*
PW	Project Work
D	Dissertation

PS: Please refer to the guidelines for 'Modes of Evaluation for Various Types of Papers', and *viva voce* nomenclature & scope and constitution of the *viva-voce* boards.

Note: The electives offered are at the discretion of the Head of the Department.

** The Project Work topic would be finalized by the end of the second semester, and the Project Work starts thereafter, continues in the third semester and gets completed in the fourth semester. The Project Work done in the third semester is reviewed based on a preliminary report submitted by the student and is evaluated for 50 marks: which is later included as part of the total marks of 250 in the fourth semester.

*** Total marks for the Project Work would be **250 marks**, which would include **50 marks** for the review of the preliminary report submitted by the student at the end of the 3rd semester (please see**) + 50 marks for the Project Work *viva-voce* conducted at the end of the 4th semester + 150 marks for the double evaluation of the Project Report submitted at the end of the fourth semester.

Credits

The elective papers are listed below:

Elective Papers offered in the Fourth Semester

FOURTH SEMESTER (Choose any ONE paper from each of the Electives listed below):

ELECTIVE – I

PCHM-404 E-I (i)	Environmental Chemistry
PCHM-404 E-I (ii)	Functional Materials
PCHM-404 E-I (iii)	Photophysics of Organic Molecules

ELECTIVE – II

PCHM-405 E-II (i)	Biocatalysis for Industry and Environment
PCHM-405 E-II (ii)	Organic Chemistry of Natural Products
PCHM 405 E-II (iii)	Advanced Aspects of Polymer Chemistry

NOTE: The students of the department may choose two electives in the fourth semester (one each from Electives-I & II) out of the elective courses listed above, under the guidance and recommendation of the Head of the Department.

PCHM-101(i): Quantum Chemistry and Group Theory
(3 CREDITS – 42 Hours)
Course Objectives:
1. To teach the fundamentals of Quantum Chemistry like the concept of Operators, Eigenvalues, Eigenfunctions etc. 2. To set up and solve the Schrodinger equation in simple systems like particle in a potential-free box, harmonic oscillator, rigid rotator and single electron systems such as hydrogen atom. 3. To introduce approximation techniques and their application to multi-electron systems. 4. To understand different molecular symmetry operations and use them to derive character tables of simple point groups. 5. To teach principles of group theory and their use in applications such as hybridization, normal mode analysis (linear and non-linear molecules) and molecular spectroscopy.
Course Outcomes: Upon completion, the student will be able to
1. Understand the fundamentals of quantum mechanics such as the concept of Operators, Eigenvalues, Eigenfunctions etc. 2. Set up Schrodinger equation and solve it for simple systems. 3. Determine the various symmetry operations for diverse molecules and use the point group character tables in the study of electrical, optical and magnetic properties. 4. Calculate the delocalization energy. 5. Identify the normal modes of vibrations for different bands in IR and Raman spectra of different molecules (linear and non-linear).
Syllabus:

1. Birth of Quantum Mechanics
Black Body Radiation, Stefan's Boltzmann Law, Wien's Displacement Law, Planck's Distribution Law, Dulong and Petit Law -2 hours
Photoelectric Effect, Hydrogen Atomic Spectrum, Bohr's Atomic Model, Wave-Particle Duality, Heisenberg Uncertainty Principle, Quantization -1 hour

2. Introduction to Quantum Mechanics
Wave equation in 1-D and 2-D, Schrodinger Wave Equation – Time Dependent and Time Independent and its Interpretation (Born's) -1 hour
Concept of operators – Linear operators, Eigenvalue Problem, State Function -1 hour
Normalization of wave function, Expectation Value -1 hour
Postulates of Quantum Mechanics -1 hour
Operator Algebra, Hermitian Operators, Commutative Operators -2 hours

3. Time-Dependent Quantum Mechanics
Light-Matter Interaction, Time-Dependent Schrodinger Equation -1 hour

4. Applications of Quantum Mechanics
Particle in 1-D Box with Infinite Potential Boundaries -1 hour
Particle in 3-D Box -1 hour
Harmonic Oscillator – Model for Diatomic Model, Formulation of Schrodinger Equation and Solution - Wave Function and Energy Levels, Hermite Polynomials, Overtones, Selection rules, Tunnelling -3 hours
Rigid Rotor - Model for Rotating Diatomic Molecule, Formulation and Solution of Schrodinger Equation- Wave Function and Energy Levels, Spherical Harmonics, Selection Rules, Non-Rigid Rotor -3 hours

5. Hydrogen Atom

Hydrogen Atom, Formulation of Schrodinger Equation and Solution, Electronic Levels, Bound State Hydrogen Atom Wave Functions -2 hours

Shapes of 1s, 2s, 2p, 3s, 3p, 3d Orbitals, Radial Distribution Functions, Born-Oppenheimer Approximation -1 hour

Term Symbols -1 hour

Effect of Spin-orbit coupling on hydrogen atom energy levels, Schrodinger Equation for Helium Atom -1 hour

6. Approximate Methods

Variation Method – Trial Functions – Linear and Nonlinear

Perturbation Method – Introduction, First Order Perturbation Theory, Second order Perturbation Theory -3 hours

7. Many Electron Atoms

Atomic Units; Hartree Method, Hartree-Fock Method Wave Functions for Helium Atom Solution by Self-Consistent Field Method, Anti-Symmetrization of Wave Functions, Slater Determinants, Correlation Energy -3 hours

8. Electronic Structure of One Electron and Many Electron Diatomic Molecules

Valence Bond Theory and Molecular Orbital Theory - Application to Hydrogen Molecule Ion, H_2^+, Hydrogen molecule, H_2, Comparison of MO and VB theories -2 hours

Huckel Π Electron Theory and its Application to Ethylene, Butadiene and Benzene -2 hours

9. Molecular Symmetry and Group Theory

Symmetry elements and Symmetry operations -1 hour

Elementary properties of groups, Sub-groups, Classes, Generator -1 hour

Point groups-classification -1 hour

Matrix form of symmetry operations, Great orthogonality theorem (Qualitative) -1 hour

Irreducible and reducible representations, Bases of representation -1 hour

Character tables (C_{2V},C_{3V}, C_{2h} in particular). -2 hours

Understanding the character table-Reduction Formula-Vanishing Integral Rule. -2 hours

REFERENCES

PRESCRIBED BOOKS:

1. Donald A. McQuarrie, Quantum Chemistry, 2nd Ed., University Science Books, California, 2008.
2. Ira N. Levine, Quantum Chemistry, 7th Ed, Prentice Hall 2013.
3. Peter Atkins, Julio de Paula, James Keeler, Physical Chemistry, 11Ed., Oxford University Press, 2018.
4. F. A. Cotton, Chemical Applications of Group Theory, 3rd Ed., Wiley 1994.
5. K. Veera Reddy, Symmetry and Spectroscopy of Molecules, New Age International (P) Ltd., Publishers Second Revised Edition 2009.

REFERENCE BOOKS:

1. P. W. Atkins and R. S. Friedman, Molecular Quantum Mechanics, 5th Ed., Oxford Univ. Press, 2010.
2. S. F. A. Kettle, Symmetry and Structure, 3rd Ed., Wiley 2007.
3. R. K. Prasad, Quantum Chemistry, 3rd Ed., Wiley Eastern, 2006.
4. K.V. Raman, Group Theory and its Applications to Chemistry, McGraw Hill Education, 1990.

PCHM-101(ii): Mathematics for Chemistry

(Non-Credit Course-28 Hours)

Course Objectives:

1. To formulate problems in applied sciences using mathematics and find solutions to them.
2. To revise and update the student with mathematical concepts applicable to chemistry like matrices, Eigenvalue problems and differential equations to solve the Schrodinger equation.
3. To equip the student with various mathematical skills for future

Course Outcomes: Upon completion, the student will be able to

1. Use mathematical tools of linear algebra and ODEs in various disciplines of chemistry confidently.
2. Apply matrix algebra in linear equations, to solve problems in chemistry.
3. Use mathematicsand probability for any given scientific challenge.

Syllabus:

1. Introduction to numbers (real numbers, complex numbers)	-2 hours
2. Functions: properties of functions-operations on functions-Dirac delta function	-2 hours
3. Series and limits	-2 hours
4. Calculus: Basics of differentiation, Basics of integration,	-2 hours
5. Differential equations	-4 hours
6. Determinants and Matrices: Matrix operations-properties of matrices	-5 hours
7. Operators: Linear Operators-Hermitian operators	-2 hours
8. Coordinate Transformation: Cartesian, Spherical and Cylindrical	-2 hours
9. Vectors: Introduction to vectors-vector operations-vector space-basis vectors-linear transformations-orthogonality properties	-3 hours
10. Matrix Diagonalization, Eigenvalues and Eigenfunctions	-2 hours
11. Probability	-2 hours

There shall not be any external examination for this mathematics course.

References:

Prescribed Textbooks

1. Donald A. McQuarrie, Quantum Chemistry, 2nd Ed., University Science Books, California, 2008.
2. George Turrell, Mathematics for Chemistry & Physics, Academic Press (2001)
3. Donald A. McQuarrie (Author), Mervin Hansen (Illustrator), Mathematics for Physical Chemistry, University Science Books (2008)

Reference Textbooks

1. Erich Steiner, The Chemistry Maths Book, Oxford University Press (2008)
2. Paul Monk, Maths for Chemistry: A Chemist's Toolkit of Calculations, Oxford University Press (2006)
3. Robert G Mortimer, Mathematics for Physical Chemistry, 3 Ed., Academic Press (2005)
4. Jay Martin Andersen, Mathematics for Quantum Chemistry, Dover Publications (2005)

PCHM-102: Analytical Chemistry

(3 CREDITS - 42 Hours)

Course Objectives:

1. To highlight the unique perspectives that analytical chemists bring to the study of Chemistry
2. To understand the statistical treatment of experimental data.
3. To study various separation techniques such as solvent extraction, chromatography crucial for both qualitative and quantitative analysis of samples.
4. To extend existing analytical methods for various samples, and to learn about their applications in the areas of radioanalytical chemistry and photoelectron chemistry.
5. To study the layout of different instruments and their components.

Course Outcomes: Upon completion, the student will be able to

1. Understand the theoretical principles behind the analytical techniques.
2. Learn important analytical techniques to analyze and separate various samples at macro and microscale.
3. Realize the applicability, advantages, and disadvantages of each method studied.
4. Gain knowledge of the layout and working of different instruments.

Syllabus:

1. Evaluation of Analytical Data:
The uses of Statistics –the standard deviation of computed results - Method of least squares, Methods for reporting analytical data, Confidence intervals, Introduction to Error Analysis, methods of detection,– P-test -3 hours

2. Separation Techniques:

Supercritical fluid chromatography- Principle and instrumentation-Applications of SCF	-2 hours
Supercritical extraction chromatography: Principles, advantages and applications	-2 hours
Capillary electrophoresis - Capillary electro-chromatography-	-2 hours
Solvent extraction - Multiple batch extraction –	-2 hours
Countercurrent distribution	-2 hours
Solid phase extraction - flow injection analysis - reverse osmosis, electrodialysis.	-3 hours
Affinity chromatography	-1 hour
Ultra High Performance Liquid Chromatography (UHPLC)	-1 hour
Pyrolysis gas chromatography; Fast Protein Liquid Chromatography	-2 hours

3. Instrumental Methods:

Different types of electrodes – mercury electrodes, solid electrodes, Chemically modified electrodes and microelectrodes-	-1 hour.
Voltammetry - pulse voltammetry (normal, differential, square wave, staircase voltammetry), AC voltammetry, - chronoamperometry-bi-amperometry	-3 hours
Cyclic Voltammetry	-2 hours
Stripping Methods (anodic, cathodic, adsorptive) and applications)	-2 hours

4. Radio-analytical Methods:

Principle of Radio analytical methods- Isotope dilution analysis	-2 hours
Radiometric titrations – precipitation and complex formation titrations	-2 hours

5. Photo-electrochemistry and Electrochemiluminescence:

Introduction to Photo-electrochemistry at semiconductor electrodes	-2 hours
Photoemission from metal electrodes - Electrochemical monitoring of photolytic intermediates - Electrochemiluminescence	-2 hours

6. Instrumentation:

Luminescence, NMR, Mass spectrometer	-4 hours
Atomic absorption spectrometry – flame photometry-principles and applications	-2 hours

References:

PRESCRIBED BOOKS:

1. D. A. Skoog, F. J. Holler and T. A. Nieman, Principles of Instrumental Analysis, 7th Ed., Saunders College publishing 2017.
2. P. T. Kissinger and W. R. Heineman, Laboratory Techniques in ElectroAnalytical Chemistry, 2nd Ed., Marcel Dekker Inc. New York 2016.
3. Stanley R Crouch, Douglas A. Skoog, F. James Holler, Donald M. West, Fundamentals of Analytical Chemistry, 9th E, Year: 2013. ISBN: 9788131522691
4. G. D. Christian, Analytical Chemistry, 7th Ed. John - Wiley & Sons 2013.
5. Joseph Wang, Analytical Electrochemistry, 3rd E, Wiley VCH, 2006.
6. J. Tolgyessy and M. Krys, Radio Analytical Chemistry Vol I & II, Ellis Horwood Ltd, 1989

REFERENCE BOOKS:

1. R. A. Day Jr., A.L. Underwood, Qualitative analysis, 6th Ed., Prentice Hall of India, 1991.
2. Vogel's Textbook of Quantitative Inorganic Analysis (revised copy), 5th Ed., ELBS, 1994.

PCHM-103: Coordination Chemistry
(3 CREDITS - 42 Hours)
1. Course Objectives:
2. To understand the key theories of coordination compounds including the energy level diagrams of different systems. 3. To be able to use the theories of metal-ligand bonding to understand the spectral and magnetic properties of coordination compounds. 4. To understand the kinetics and reaction mechanisms involving octahedral and square planar metal complexes. 5. Introduce the underlying concepts behind the photochemistry of coordination compounds.
Course Outcomes: Upon completion, the student will be able to
1. Understand the splitting of 'd' orbitals of transition metals in the presence of a crystal field, and their energies (Octahedral, tetrahedral, and square planar). 2. Explain the origin of colours in various coordination compounds. 3. Calculate ligand-field stabilization energies.
Syllabus:
1. Theories of Metal-Ligand Bonding: Crystal field theory: Important aspects of crystal field theory - -1 hour d-orbitals splitting in octahedral, tetrahedral, square planar, square pyramidal and trigonal bipyramidal geometries – -2 hours 10Dq value and its calculation - CFSE in weak field and strong field cases -1 hour Factors affecting magnitude of 10Dq - Spectrochemical series – -1 hour Jahn-Teller Theory-applications of crystal field theory (colour and magnetic properties of complexes) Limitations of crystal field theory -2 hours Molecular Orbital theory: Formation of molecular orbitals by LCAO method - Nephelauxetic effect -2 hours MO energy level diagrams for octahedral, tetrahedral and square planar complexes involving only σ bonding and σ and Π bonding -2 hours Measurement of pi-bonding effects -1 hour **2. Study of Complexes in Solution:** Introduction to stability constants -1 hour Factors affecting stability constants - Kinetic and thermodynamic stability - Irwin-William series -1 hour Concept of Hard and Soft acids and bases -1 hour Methods of determining stability constants (spectrophotometric, conductometric and pH-metric methods) -1 hour **3. Electronic Spectra of Metal Complexes:** A term symbol gives a detailed description of an electron configuration-allowed values of J -1 hour Hund's rules are used to determine the term symbol of the ground electronic state-atomic term symbols are used to describe atomic spectra, Term symbols of d^n ions -1 hour

Russel –Saunders coupling is most useful for light atoms -1 hour
Spectra of transition metal ions – Orgel diagrams for d^2 to d^9 octahedral and tetrahedral complexes -2 hours
Tanabe - Sugano diagram for d^2 ion complex -1 hour
Charge transfer transitions - Selection rules and transition probabilities based on symmetry considerations. -1 hour

4. Magnetic Properties of Complexes:
Types of magnetism (dia, para, ferro and antiferromagnetism) - Temperature independent para-magnetism -1 hour
Magnetic susceptibility and its determination by Gouy and Faraday methods -1 hour
Calculation of magnetic moment from magnetic susceptibility -1 hour
Spin-orbit coupling and its effect on magnetic moments -1 hour
Orbital contribution to magnetic moment-single molecule magnets -1 hour

5. Kinetics and Mechanisms of Reactions:
Inert and labile complexes-substitution reactions in octahedral and square planar complexes -1 hour
D, I_d, I_A and A mechanisms -1 hour
Bond making and Bond breaking- The Langford- Gray nomenclature- -1 hour
Coordination number and substitution mechanisms- Stereochemistry of substitution- -2 hours
Effect of non-participating ligands on the stability of complexes. Trans-effect in square - planar complexes -2 hours
Theories of Trans-effect (Polarization and pi-bonding theories)- Quantitative aspects of the Trans effect -1 hour
Dissociation mechanism-Substitution of non- coordinating and coordinating solvents - Electron transfer reactions: Inner and outer sphere mechanisms -2 hours
Marcus Cross relationship - Template effect -1 hour

6. Photochemistry of Coordination Compounds:
Introduction to Photochemical reactions - Laws of Photochemistry - Excited states of metal complexes -1 hour
Photo-substitution, photo-dissociation -1 hour
Photo-oxidation, Photo-reduction and Photo-isomerisation reactions of complexes -1 hour

References:

Prescribed Books:

1. Asim. K. Das, Fundamental Concepts of Inorganic Chemistry, 3rd Ed., (volumes: 1-7), CBS Publishers and Distributors Pvt. Ltd., 2020.
2. J.E. Huheey, E.A. Keiter and R.L. Keiter, Inorganic Chemistry, 4th Ed., Pearson, 2013.
3. F.A. Cotton and G.W. Wilkinson, Advanced Inorganic Chemistry, 6th Ed., John Wiley, 1999.
4. D. Banerjea, Coordination Chemistry, 3rd Ed., Tata-McGraw-Hill 2009.
5. David Nicholls, Complexes and First Row Transition Elements, Macmillan 2017.
6. O. Kahn, Molecular Magnetism, Wiley VCH, 1993.
7. Martin L. Tobe and John Burgess, Inorganic Reaction Mechanisms, Longman, 1999.

Reference Books:

1. V. Balzani& V. Carasiti, Photochemistry of Coordination Compounds, Academic Press, New York 2007.
2. B. Douglas, D.H Mc Daniel & J.J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Ed., John Wiley, New York 1997.
3. M. Gerloch& E.C Constable, Transition Metal Chemistry, VCH Publications New York, 1994.
4. R. G. Wilkins, Kinetics and Mechanisms of Reactions of Transition Metal Complexes, 2nd Ed., VCH publications, 1991.
5. F. Basolo and R. G. Pearson, Mechanisms of Inorganic Reactions, 2nd Ed., Wiley Eastern, 1977.
6. Robert B. Jordan, Reaction mechanisms of Inorganic and Organometallic systems, 3rd Ed; Oxford University Press, Oxford, 2007.
7. Gary Wulfsberg, Inorganic Chemistry, University Science Books, California, 2000.
8. Issac B Bersuker, Electronic Structure and Properties of Transition Metal Compounds, 2nd Ed., Wiley, 2010.

PCHM-104: Advanced Aspects of Organic Structure and Stereochemistry

(3 CREDITS - 42 Hours)

Course Objectives:

1. To provide an understanding of aromaticity, non-aromaticity and anti-aromaticity using Molecular Orbital Theory.
2. To elucidate the reactivity and aromaticity in heterocyclic compounds.
3. To give an in-depth understanding of the conformational studies in cycloalkanes supplemented by NMR spectral analysis. This also includes stability studies of trans annular reactions.
4. To provide an idea of optical isomerism in organic molecules and application of chiro-optical methods for configurational studies.

Course Outcomes: Upon completion, the student will be able to

1. Identify and predict the aromaticity of organic molecules.
2. Solve numerical problems related to aromatic and antiaromatic systems.
3. Predict and identify the stability and optical activity of any organic molecule, having got a strong background in the stereochemical aspects of conformation and configuration.

Syllabus

1. Delocalization, Resonance and Aromaticity:

Delocalized Chemical Bonding, Molecular Orbitals of Benzene -1 hour

Molecules that have Delocalized Bonds-Double Bonds in Conjugation-Butadiene -1 hour

Cross conjugation-Structure and Chemistry of Dendralenes and Radialenes -1 hour

Rules of Resonance, Resonance Effect and ylids -1 hour

Aromaticity-Six membered rings -1 hour

Five Seven and Eight Membered Rings-Cyclopentadienyl carbanion, Cycloheptatrienyl carbocation - tropone and tropolones, Heteroaromatic compounds -1 hour

Other Systems containing Aromatic Sextets: Azulenes, Fulvenes and Fulvalenes -1 hour

Alternant and Non-Alternant Hydrocarbons -1 hour

Aromatic Hydrocarbons with Electron Numbers Other than Six- Systems of Two electrons-The cyclopropenyl carbocation -1 hour

Systems of four electrons-Antiaromaticity of cyclobutadiene; Systems of Eight electrons-Cyclooctatetraene -1 hour

Systems of 10 electrons; Systems of more than 10 –electrons (4n + 2)- upto [18]Annulene; Systems of more than 10 electrons: (4n) upto [16] Annulene. -1 hour

Dewar's perturbation of molecular orbitals approach to the prediction of aromaticity, non-aromaticity and anti-aromaticity of conjugated cyclic systems. -1 hour

Different criteria for aromaticity and different methods for determining aromatic character -Huckel's rule - Mobius system -1 hour

Other Aromatic compounds: Mesoionic compounds-sydnones, Homoaromatic compounds, the chemistry of fullerenes with particular reference to Buckminsterfullerene (C60). Determination of structure, reactions and applications -1 hour

Less-common conjugative interactions such as hyperconjugation and homo-conjugation - evidence and illustrative examples. -1 hour

Tautomerism: Keto-Enol Tautomerism and other Proton Shift Tautomerism -1 hour

An introduction to computer assisted energy calculations of aromatic, anti-aromatic and non-aromatic systems using ab initio molecular orbital packages/programs -1 hour

2. Valence bond tautomerism and rigid structures:

Explanation of the phenomenon of valence - bond tautomerism fluxional molecules illustrated by homotropylidene and bullvalene. -1 hour

3. Conformational Analysis:

Conformations of cyclic compounds - small ring systems (Cyclopropane, Cyclobutane and Cyclopentane) - a review. -1 hour

Conformations of cyclohexane and cyclohexanone, and monosubstituted cyclohexanes disubstituted cyclohexanes - Conformational and configurational isomerism - Relative order of stabilities - preferred conformations -2 hours

Conformational analysis of cyclohexanes - Dynamic aspects- typical reactions which bring out the differences between stereoisomers -2 hours

Electrophilic and Nucleophilic additions in Substituted cyclohexene and cyclohexane epoxide systems -1 hour

Medium - size ring systems - Conformations of Cyclopentane, Cyclooctane, and Cyclononane -1 hour

Conformations of cyclodecane - transannular reactions with particular reference to the cyclodecane system -2 hours

Bicyclic compounds with particular reference to decalin -1 hour

Strained bicyclic systems -1 hour

Application of NMR spectral data (coupling constants in conformational analysis and introduction to NOE-application in stereochemistry) -2 hours

4. Advanced aspects of configurational isomerism:

Sequence rule and its applications to a wide range of situations -1 hour

Stereochemistry of compounds containing two and more unequal chiral centers - Concept of pseudo-chirality -1 hour

Stereochemistry of allenes and spiranes -1 hour

Optical isomerism due to restricted rotation. Atropisomerism, Isomerism exhibited by Biphenyls -1 hour

Further examples of atropisomerism - polyphenyls, "Ansa" compounds, "paracyclophanes" and hexahelicene. Akampt isomerism -1 hour

Determination of absolute configuration - chemical interconversions - classical examples of (+) tartaric acid, (-) Lactic acid and related compounds -1 hour

Chemical correlations involving diastereoisomers - Determination of the absolute configuration of Shikimic acid -1 hour

Configurational assignments based on asymmetric synthesis - Applications of Cram's rule and Prelog's rule - illustrative examples -1 hour

Chiro-optical methods-principles of optical rotatory dispersion and circular Dichroism -1 hour

Applications of the O.R.D. and C.D techniques - plain and cotton effect curves- Study of conformations and configurations of organic molecules and CD of protein and peptide conformations -1 hour

The alpha - halo - ketone rule, octant rule and their applications -1 hour

References
PRESCRIBED BOOKS: 1. Michael B. Smith, March's Advanced organic chemistry, 7th Ed., John Wiley & Sons Inc., New York, 2016. 2. J. Clayden, N. Greeves, S. Warren, Organic chemistry, 2nd Ed., Oxford University Press, 2012. 3. R. A. Y. Jones, Physical and Mechanistic Organic Chemistry, 2nd Ed., Cambridge University Press, 1984. 4. William J. Le Noble, Highlights of Organic Chemistry, Marcel Dekker Inc. New York, 1974. 5. E. L. Eliel, Stereochemistry of carbon compounds, Tata Mc Graw Hill, 1975. 6. D. Nasipuri, Stereochemistry of organic compounds principles and applications, New Age International (P) Limited, 4th Ed, 2021. **REFERENCE BOOKS:** 1. J. A. Marshall, Carbon-Carbon and Carbon - Proton NMR couplings - Applications to Organic Stereo-chemistry and Conformational Analysis, Florida Verlag Chemie, 1983. 7. Fullerenes, Ed George S Mammond, Valerie J Cook, ACS Symposium Series, 4 :1, 1982.

PCHM-105: Practical: Coordination Chemistry (Preparation and Analysis)
2 CREDITS
Course Objectives:
1. To prepare inorganic coordination complexes of different transition metals with ligands of various types. 2. To estimate the metal content of these complexes by standard analytical methods. 3. To familiarize the student with the know-how of the procedure to record spectra using various instruments and interpret them. 4. To characterize the prepared metal complexes. 5. To learn various methods to determine the metal-ligand stoichiometry in metal complexes.
Course Outcomes: Upon completion, the student will be able to
1. Prepare metal complexes of different transition elements with various types of ligands. 2. Estimate the metal content of the complexes by standard analytical methods. 3. Record and interpret the absorption spectra and IR spectra of various coordination complexes. 4. Determine the metal-ligand stoichiometry in metal complexes.
Syllabus:
1. **Metal Complex Preparation:** Preparation of Hexammine Nickel(II) chloride 2. **Metal Content Determination by AAS/MPAES:** Hexammine Nickel(II) chloride 3. **Electronic Spectroscopy of Metal Complexes:** Recording absorption spectrum of a metal complex in solution and analyzing it 4. **Infrared Spectroscopy of Metal Complexes:** Characterization of Dichlorobis(triphenylphosphine)nickel (II) complex using Infrared spectroscopy 5. **Formation Constant Measurement:** Determination of the formation constant of iron (III) salicylate complex 6. **Stoichiometry Determination by Job's Method of Continuous Variation:** Spectrophotometric determination of stoichiometry of Iron-phenanthroline complex by Job's Method of continuous variations 7. **Molecular Formula Determination by Mole-Ratio Method:** Spectrophotometric determination of molecular formula of Zirconium-Alizarin Red-S complex by Mole-ratio method 8. **Metal- Ligand Ratio Determination:** Spectrophotometric determination of metal-ligand ratio in Copper-Ethylenediamine complex: Slope-ratio method 9. **Photochemistry Experiment:** Potassium Trioxalatoferrate III: Synthesis and photochemistry 10. **Electrochemical Studies:** Obtaining a cyclic voltammogram of a metal complex and analyzing it 11. **Band Gap Determination:** Determination of band gap of materials using diffuse reflection spectroscopy (Tauc plot) 12. **His Tag Affinity Chromatography:** Separation of molecules containing imidazole groups from molecules without them **Note:** Minimum of 8 experiments to be carried out.
References:

1. A. I. Vogel, A Textbook of Quantitative Inorganic Analysis, 5th Ed., Longman, 1989.
2. G. Pass and H. Sutcliffe, Practical Inorganic Chemistry, 2nd Ed., Science Paperbacks, 1979.
3. J. Derek Woolins, Inorganic Experiments, Ed., 3rd Revd. Ed., Wiley-VCH, 2010.
4. O. P. Vermani& A. K. Narula, Applied Chemistry (Theory & Practice), 2nd Ed., Wiley Eastern, 2017.

PCHM-106:Practical: Analytical Chemistry

2 CREDITS

Course Objectives:

1. To enrich the student with faculties to apply the conceptual analysis of fundamental principles in the implementation for diverse analytical chemical systems.
2. To introduce different analytical instruments for the determination of analytes of varied nature, from millimolar to micromolar concentrations.
3. To introduce different electro-analytical techniques of varied industrial and academic importance.

Course Outcomes: Upon completion, the student will be able to

1. To design experiments with better sample preparation for accurate analysis.
2. To handle sophisticated equipment for different chemical analysis.

Syllabus:

1. Potentiometric determination of permanganate in pyrophosphate
2. Conductometric estimation of H_2SO_4, CH_3COOH and $CuSO_4$
3. Differential pulse voltammetric analysis of trace ions present in natural samples
4. Synthesis and characterization of silver nanoparticles of different shapes and sizes and their utility in environmental dye degradation studies
5. Titrimetric analysis based quantitative determination of halides in mixtures
6. Quantitative analysis of nitrates and sulphates using Ion chromatography
7. Qualitative Identification of mixture of compounds using HPLC
8. Quantitative analysis of a mixture of compounds using GC
9. Quantification of Caffeine/Polyphenols in various teas using HPLC
10. Estimation of Fluoride ion using Ion selective electrode.
11. Estimation of Ca and Mg from the mixture of their respective oxalate using TGA
12. Estimation of trace metal content in environmental samples using MP-AES

Note: Minimum of 8 experiments to be carried out.

References:

1. Donald T. Sawyer, William R. Heineman &Jalice M. Beebe, Chemistry experiments for Instrumental Methods, John Wiley & Sons, 1991.
2. Vogel's Textbook of Quantitative Chemical Analysis (revised copy) 5th Ed., ELBS, 1994.
3. G. Peter Matthews, Experimental Physical Chemistry, Clarendon Press, 1985.

PCHM-107: Practical – Organic Qualitative Analysis
(Mixture Separation, Functional Group Analysis and Drug Analysis)

2 CREDITS

Course Objectives:

1. To develop skills to separate binary mixtures of different classes of organic compounds and identify functional groups present in the individual components.
2. To confirm the presence of functional groups through derivative preparation.
3. To use Thin-Layer Chromatography for analysis of simple APIs available in the market.
4. To practice column chromatography for the separation of binary and ternary mixtures of organic compounds.

Course Outcomes: Upon completion, the student will be able to

1. Separate binary organic mixtures and identify functional groups in the individual compounds.
2. Apply the techniques learnt to separate and analyse organic compound mixtures obtained during synthesis.

Syllabus:

1. Separation of binary mixtures
Separation of binary mixtures comprising aliphatic and/or aromatic organic compounds with functional groups such as alcohols, acids, amines, carbohydrates, esters, ethers, nitro, ketones, aldehydes, hydrocarbons, halogen derivatives followed by their characterization using qualitative functional group analysis and derivative preparation – *5 mixtures to be separated and analyzed (3 hours each)*
(Separation methods include extraction using $NaHCO_3$ (aq.), extraction using NaOH (aq.), extraction using HCl (aq.), extraction using ether, and distillation)

2. TLC Analysis
Preparation of TLC plates
TLC analysis of some medicines.

3. Column Chromatography based separation
Separation of binary and ternary mixtures of organic compounds using column chromatography.

4. Paper Chromatography
Separation of chlorophyll or dyes

References:

1. V K Ahluwalia and S Dhingra, Comprehensive Practical Organic Chemistry – Qualitative Analysis, University Press, India 2000.
2. A.I Vogel, Elementary Practical Organic Chemistry Part II, Qualitative Organic analysis, 2nd Ed, CBS publications, 1987.
3. C. M. Garner, Techniques and Experiments for Advanced Organic Laboratory, John Wiley and Sons, 1997
4. Egon Stahl, Thin Layer chromatography – Laboratory Workbook edited, Springer International student edition, 1969.

5. Raphael Ikan, Chromatography in Organic micro-analysis – A laboratory guide, Academic press, 1982.
6. P.D. Sethi, Quantitative analysis of Drugs in Pharmaceutical preparations, 3rd Ed., CBS publishers, 1997.
7. P.R. Singh, D.S. Gupta and K.S. Bajpai, Experimental Organic Chemistry, Vols I & II, Tata Mc Graw Hill, 1980.

PCHM-201: Structural Inorganic and Bio-Inorganic Chemistry
(3 CREDITS – 42 Hours)
Course Objectives:
1. To study the synthesis, structure, bonding and reactions of various inorganic compounds. 2. Study the role of trace metals in biological systems. 3. To study the structure and function of various metalloenzymes. 4. To understand the mechanism of action of metalloenzymes in various biologically important functions.
Course Outcomes: Upon completion, the student will be able to
1. Have the knowledge of synthesis, structure, bonding and reactions of various inorganic compounds. 2. Understand the role of different trace metals present in biological systems. 3. Overview of structure and functions of important metalloenzymes. 4. Know the mechanism of metalloenzymatic activity in various biologically important functions.
Syllabus:

Structural Inorganic Chemistry:
1. Synthesis, Reactions, Structure and Bonding in:

Catenated compounds: Catenation –Heterocatenation, Intercatenation	-2 hours
Isopoly Anions and Heteropoly anions.	-2 hours
Ring compounds. Borazines - Phosphazenes, Polyphosphazenes sulfur nitrogen rings and other Heterocyclic systems	-2 hours
Homocyclic inorganic ring systems (S, Se & P and oxocarbon anions).	-2 hours
Cage compounds: Phosphorous cage compounds with oxygen, sulfur and arsenic atoms	-1 hour
Boron cage compounds: Boranes, Synthetic strategies in Boron cage chemistry, Pharmacologically active Boron analogues of amino acids,	-2 hours
The Pyrazoboles, Carboranes and Metallocarboranes.	-1 hour
2. Inorganic polymers: Synthesis, structure and applications of the polymers	
Polyphosphazenes,	-1 hour
Polysilanes	-2 hours
Polysiloxanes	-1 hour
Metal chelate polymers	-1 hour
Inorganic polymers that contain phosphorus, Boron and Sulphur	-1 hour
3. Bio-Inorganic chemistry:	
New perspectives and biological roles of essential trace elements	-1 hour
4. Oxygen Carriers: Transport and storage of dioxygen.	-1 hour
Reactions of dioxygen- structure and functioning of hemoglobin and myoglobin	-1 hour
Hemerythrins Hemocyanin	-1 hour
Model compounds for oxygen carriers (Vaska's iridium complex, cobalt – DMG complex)	-1 hour
5. Biological Nitrogen Fixation: Nitrogen fixing organisms – structure and function of nitrogenase enzyme – Chemistry of nitrification	-1 hour
Fixation via nitride formation	-1 hour
Dinitrogen complexes as biological models	-1 hour

6.Metalloproteins – Metalloenzymes: The characterization of metal – binding sites	-1 hour
Carbonic anhydrase – Carboxypeptidase	-2 hours
Superoxide dismutase – Structure and biochemical functions of B_{12} Coenzyme	-1 hour
Selenium and sulphur containing bio-molecules	-1 hour
Zinc fingers and Calmodulins	-1 hour
Introduction to Iron-Sulphide complexes, Catalase, Succinate hydrogenase, NADH dehydrogenase	-1 hour
7. Alkali Metal Transport in Biological Systems:	
Introduction – Coordination chemistry of alkali metal ions	-1 hour
Ion transport – Modes of passage	-1 hour
Sodium-dependent transport.	-1 hour
8. Metal Ions Toxicity and Chelation Therapy:	
Toxicity of metal ions particularly heavy metal ions –	-1 hour
Chelating agents-chelation therapy	-1 hour
Therapeutic uses of metals, ligands and complexes with special reference to anti-cancer activity	-2 hours
9. Metal Ion Folding and Cross-linking of Biomolecules:	
Metal-ion stabilization of protein structure and nucleic acid structure	-1 hour
Protein binding to metallated DNA	-1 hour

References:

PRESCRIBED BOOKS:

1. J. E. Huheey, E. A. Keiter and R. L. Keiter, Inorganic Chemistry, Harper Collins, 4th Ed., Pearson, 2013.
2. F.A. Cotton and G. Wilkinson, Carlos A. Murillo, Manfred Bochmann, Advanced Inorganic chemistry, John Wiley, 6th Ed., New York, 2021.
3. N.N. Greenwood and A. Earnshaw, Chemistry of the elements, 2nd Ed., Butterworth- Heinemann, 1997.
4. J.E. Mark, H.R. Allcock and R. West, Inorganic Polymers, Prentice Hall, 1992.
5. Wolfgang Kaim and B. Schwederski, Bioinorganic Chemistry, John Wiley, New York, 1994.
6. J. A. Cowan, Inorganic Biochemistry – An Introduction, VCH, 1993.
7. S. J. Lippard and J. M. Berg, Principles of Bioinorganic Chemistry, University Science Books, California, 1994.

REFERENCES BOOKS:

1. Reenberg and R.E. Williams, Advances in Boron and the Boranes, VCH, 1988.
2. Vadapalli Chandrasekhar, Inorganic and Organometallic Polymers, Springer, 2005.
3. M.N. Hughes, Inorganic Reactions of biological processes, John-Wiley, 2nd Ed., New York 1981

PCHM-202: Chemical Kinetics and Surface Chemistry
(3 CREDITS – 42 Hours)
Course Objectives:
1. To develop an understanding of the theories of reaction rates. 2. To develop an understanding of the study of chemical kinetics in elementary reactions and subsequently in systems of greater complexity. 3. Study of reaction mechanisms using chemical kinetics. 4. To study the kinetics of catalytic reactions, photochemical reactions, chemical reactions and fast reactions. 5. To develop an understanding of the chemistry of surfaces, physisorption, chemisorption, and of the electrical double layer.
Course Outcomes: Upon completion, the student will be able to
1. Analytically approach problems of chemical kinetics. 2. Appreciate usage of model systems as tools for problem-solving. 3. Solve numerical problems related to systems studied. 4. Apply techniques, such as photoelectron spectroscopy, to carry out surface chemical analysis.
Syllabus:

Chemical Kinetics:

1. Theories of Reaction rates

Kinetic theory of collisions -1 hour
Rate theories based on thermodynamics and statistical mechanics -1 hour
Conventional transition state theory, some applications of conventional transition state theory -1 hour
Thermodynamic formulation of conventional transition state theory -1 hour
Assumptions and limitations of conventional transition state theory -1 hour

2. Elementary Gas-Phase Reactions:

Bimolecular reactions - Trimolecular reactions - Unimolecular reactions. -2 hours

3. Elementary Reactions in Solutions:

Solvent effects on reaction rates - Factors determining the reaction rates in solution -1 hour
Reactions between ions – Salt effect -2 hours

4. Composite Reactions:

Types of composite mechanisms - rate equations for composite mechanisms(Opposing, Parallel and Consecutive) -3 hours
Chain reactions: Inorganic reactions: Hydrogen – Bromine, Hydrogen - Chlorine and Hydrogen - Iodine reactions -2 hours
Organic decompositions: Goldfinger-Letort-Niclause rules - Inhibition mechanisms -1 hour
Acetaldehyde decomposition -1 hour
Gas - Phase combustion -Hydrogen - oxygen reaction. -1 hour

5. Photochemical Reactions:

Photochemical reactions - Laser photochemistry – Photosensitisation, Photophysical processes -2 hours

6. Homogeneous Catalysis:
General catalytic mechanisms - Acid-base catalysis -1 hour
Catalysis by enzymes - influence of concentration (single substrate, double substrate), inhibition -2 hours

7. Kinetic Isotope Effects:
Equilibrium, Primary and Secondary Kinetic Isotope effects -2 hours

8. Fast Reactions kinetics:
Relaxation and flow methods. Diffusion-controlled reactions. Fluorescence quenching, Common ion inhibition -2 hours
Flash photolysis and introduction to Time-resolved Pico/Femto second methods -3 hours
(e.g. introduction to Time-Correlated Single Photon Counting and FRET)

9. Reaction Dynamics:
Potential energy surfaces and classical trajectories, Concept of Saddle points -2 hours

Surface Chemistry:
10. Adsorption of Gases and Vapours on Solids:
Adsorption time - the Langmuir adsorption isotherm - kinetic derivation -1 hour
Statistical derivation of Langmuir adsorption isotherm -1 hour
Adsorption entropies - lateral interaction -1 hour
The BET and related isotherms - derivation of the BET equation - properties of the BET equation -1 hour

11. Langmuir Blodgett Films:
Structure and characterization mixed LB film, studies of the LB deposition process -1 hour

12. Chemisorption and Catalysis:
Thermodynamics of adsorption, Chemisorption - the molecular view - Chemisorption isotherms -1 hour
Kinetics of Chemisorption - The Chemisorption bond -1 hour

13. Electrical Aspects of Surface Chemistry:
Electrical double layer - Stern treatment of the electrical double layer -1 hour
Free energy of a diffuse double layer - Repulsion between two plane double layers - zeta potential -1 hour
Streaming potential and Sedimentation potential -1 hour

References:

PRESCRIBED BOOKS:

1. Peter Atkins, Julio de Paula and James Keeler, Atkins' Physical Chemistry, 11th edition, Oxford University Press, 2018.
2. K.J. Laidler, Chemical Kinetics, 3rd edition, Pearson Education Inc., 2003.
3. S. K. Upadhyay, Chemical Kinetics and Reaction Dynamics, Springer USA and Anamaya Publishers, New Delhi, 2006
4. K.A. Connors, Chemical Kinetics - The Study of Reaction Rates in Solution, – VCH Publishers, New York 1990.
5. K. J. Laidler, Physical Chemistry with Biological Application, Benjamin Cummings Publications Company Inc., Menlo Park, California 1978.

6. A.W. Adamson and A.P. Gast, Physical Chemistry of Surfaces, 6th Ed. John Wiley & Sons New York 1997.
7. J, O, M Bockris, A. K. N. Reddy, M. Gamboa-Aldeco, Modern Electrochemistry, Volume 2A – Fundamentals of Electrodics, 2nd Ed., Kluwer Academic Publishers, New York 2002.

REFERENCE BOOKS:

1. H. Strehlow and W. Knoche, Fundamentals of Chemical Relaxation, Verlag Chemie, Weinheim 1977.
2. C.D. Ritchie, Physical Organic Chemistry, The Fundamental Concepts, Marcel Dekker, Inc, 1990.
3. P.C. Hiemenz, Principles of Colloids and Surface Chemistry, 2nd edition, Marcel Dekker, INC. 1988.
4. G.D. Billing and K.V. Mikkelsen, Introduction to Molecular Dynamics and Chemical Kinetics. John Wiley & Sons 1996.
5. K.J. Laidler, Physical Chemistry of Surfaces, 3rd Ed., New Delhi, Person Education, 2016.

PCHM-203: Statistical Thermodynamics and Electrochemistry
(3 CREDITS – 42 Hours)
Course Objectives:
1. Introduce the students to the basic concepts of statistical thermodynamics. 2. Teach the concept of the partition function and its use in the calculation of various thermodynamic properties. 3. To equip the students with the ability to apply theoretical principles of electrochemistry associated with ionics and electrodics and their usage in various applications. 4. To study the applications of electrochemistry in electrocatalysis, electricity storage, photoelectrocatalysis and electrochemical sensors.
Course Outcomes: Upon completion, the student will be
1. Familiar with the postulates of statistical thermodynamics, the concept of ensemble and its types, ensemble average, ergodicity, configuration, thermodynamic probability etc. 2. Familiar with the concept of the partition function and also be able to use it for evaluation of various thermodynamic properties. 3. Able to understand the theoretical concepts behind ionics and electrodics and their usage in various electrochemical applications. 4. Able to learn and understand the concepts and principles behind various important electrochemical applications such as electrocatalysis, electricity storage, photoelectrocatalysis and electrochemical sensors.
Syllabus:

1. Introduction: Basics of Statistical Mechanics: Postulates, hypothesis and Implications
Concept of Irreversibility -2 hours

2. Probability Theory: Discrete vs Continuous, Stirling's Formula -1 hour

3. Ensembles and Distributions

Configuration and Weights/Thermodynamic Probability, Ergodicity -1 hour

Ensembles: Concept of an Ensemble, Microcanonical Ensemble, Canonical Ensemble, Grand Canonical Ensemble -1 hour

Distributions: Maxwell-Boltzmann Distribution, Bose-Einstein Distribution,
Fermi-Dirac Distribution -1 hour

Negative absolute temperature -1 hour

4. Partition Functions

Partition Function Definition - Thermodynamic Functions in Terms of the Partition Function -1 hour

The Relation of State Functions to the Partition Function -1 hour

Molecular Interpretation of the Partition Function -1 hour

Separation of Contributions

Evaluation of the Partition Function - Translational Partition Function -2 hours

Rotational Partition Function -2 hours

Vibrational Partition Function -2 hours

Electronic Partition Function - Nuclear Partition Function -1 hour

Thermodynamics of Mixing: Energy and Entropy of Binary Mixing -1 hour

Statistical Interpretation of the Equilibrium Constant -1 hour
Einstein and Debye Models of a Crystal -2 hours
Ideal lattice gas – Electron gas -1 hour

Electrochemistry
5. Ionics:
Electrochemistry of Solutions, Electrolytic Conductivity and Its Types -1 hour
Debye-Huckel Theory with Derivation -2 hours
Debye-Huckel-Onsager Treatment and Its Extension with Derivation -3 hours

6. Electrodics:
The Concept of Overpotential, Types of Overpotentials: Origin and Minimization; Exchange Current Density -1 hour
Electrochemical Reactions under Charge Transfer Control, Basic Electrodic Equation - Butler-Volmer Equation- Derivation -2 hours
The Current Potential Laws at Other Types of Charged Interfaces -1 hour
Electrode Reactions and Chemical Reactions – Multistep Reactions -1 hour
Determining the StepWise Mechanism of an Electrode Reaction -1 hour

7. Applications:
Electrodic Reactions of Special Interest – Electrocatalysis – Influence of Various Parameters. -1 hour
Photoelectrochemistry: Introduction-Band Bending at the Semiconductor/Solution Interface-Photoexcitation of Electrons by Absorption of Light-Surface Effects in Photoelectrochemistry -2 hours
Application of Butler-Volmer equation in corrosion – Tafel Equations, Determination of Kinetic Parameters -3 hours
Photoelectrocatalysis-The Photoelectrochemical Splitting of Water-The Photoelectrochemical Reduction of CO_2. -1 hour
Electrochemical Impedance Spectroscopy -1 hour

References:

PRESCRIBED BOOKS:

1. U. Fried, H. F. Hameka and U. Blukis, Physical Chemistry, Macmillan Publication, 1977.
2. Peter Atkins, Julio de Paula, James Keeler, Physical Chemistry, 11 Ed., Oxford University Press, Oxford, 2018.
3. J. O. M. Bockris and A. K. N. Reddy, Modern Electrochemistry, Volumes 1 & 2, Plenum Press, New York. 1988.
4. J. O. M. Bockris and A. K. N. Reddy, Modern Electrochemistry 2B, 2nd Ed., Kluwer Academic/Plenum Publishers, New York, 2000.
5. Allen J. Bard, Larry R. Faulkner, Henry S. White, Electrochemical methods –Fundamentals and Applications, John Wiley & Sons, Limited, 2020

REFERENCE BOOKS:

1. Robert G. Mortimer, Physical chemistry, 3rd Ed., Academic Press, 2008.
2. Normand M. Laurendeau, Statistical Thermodynamics: Fundamentals and Applications, Cambridge University Press, Cambridge, 2005.
3. John M. Seddon and Julian D. Gale, Thermodynamics and Statistical Mechanics, The Royal Society of Chemistry, London, 2002.
4. Thomas Engel, Philip Reid, Thermodynamics, Statistical Thermodynamics, & Kinetics, 4th Ed., Pearson, 2018.
5. Biman Bagchi, Statistical Mechanics for Chemists and Materials Science, CRC Press, Taylor and Francis Group, 2019.
6. J. Goodisman, Electrochemistry Theoretical Foundation, John Wiley Sons, 1987.
7. Christopher M. A. Brett, Ana Maria, Oliveira Brett, Electrochemistry: Principles. Methods and Applications, Oxford University Press, Oxford, 1993.
8. Philip H. Reiger, Electrochemistry, Prentice-Hall International, Inc., 1987.
9. Nivaldo J. Tro, Principles of Chemistry: A Molecular Approach, 4th Ed., Pearson, 2019.

PCHM-204: Physical and Mechanistic Aspects of Organic Chemistry

(3 CREDITS – 42 Hours)

Course Objectives:

1. To study detailed mechanistic aspects of nucleophilic addition reactions in carbonyl compounds, elimination reactions through E_i mechanism and aromatic substitution reactions.
2. To give a basic understanding of pericyclic reactions, molecular rearrangements and free radical reactions.

Course Outcomes: Upon completion, the student will be able to

1. Predict the products formed in the chemical reactions studied in the course with the appropriate reaction mechanism.

Syllabus:

1. Addition to the carbonyl group:

Hydride transfer reactions, stereochemistry of hydride reduction -1 hour
Clemmenson& Wolff -Kishner reductions -1 hour
Crossed and intramolecular Cannizzaro reactions -1 hour
Mechanism of benzoin condensation and crossed aldol condensations- directed aldol condensations -1 hour
Claisen and related condensation reactions -1 hour
Thorpe reaction, Stobbe condensation -1 hour
Acyloin condensation and its usefulness in the synthesis of large ring compounds -1 hour
Mannich reaction and Ritter reaction -1 hour

2. Elimination reactions:

Chugaev reaction, cleavage of quaternary ammonium hydroxides, quaternary ammonium salts with strong bases – -1 hour
Amine oxides, sulfoxides & selenium oxides -1 hour
Conversion of epoxides to olefins - Shapiro reaction - decomposition of p-toluene - sulfonyl hydrazones -1 hour
Cis - elimination - pyrolytic eliminations - Stereochemistry -1 hour
1,4 - Addition of organometallic compounds to activated double bonds -1 hour

3. Aromatic substitution reactions:

A review of the generalized mechanism - directive and rate controlling factors – Substituent effects, Partial rate factors- -1 hour
Gattermann formylation, Vilsmeier - Haack formylation and related reactions -1 hour
Nucleophilic aromatic substitution reactions going through the benzyne mechanism- and Meisenheimer complex. -1 hour
SR_{N1} aromatic substitution reactions - Aromatic homolytic substitution reactions -1 hour
Substitution reactions of thiophene, furan, pyrrole -2 hours
pyridine, pyridine oxide- quinoline and isoquinoline -2 hours
Addition reactions of furan & thiophen - Chichibabin reaction, Skraup synthesis & Fisher indole synthesis -2 hours
Modifications to Hammett equation, Brown and Taft equations -1 hour

4. Pericyclic reactions:

Electrocyclic reactions -1 hour

Cycloaddition reactions: 2+2 photochemical and-[2+2] Thermal Pericyclic reactions suprafacial and antarafacial additions -1 hour

Stereochemistry of Diels - Alder reaction -1 hour

Sigmatropic rearrangements -1 hour

Claisen, abnormal Claisen and Cope rearrangements -1 hour

FMO approach and aromatic transition state theory in pericyclic reactions

Examples and problems on pericyclic reactions -1 hour

5. Molecular rearrangements:

Benzilic acid and Demjanov rearrangements- -1 hour

Favorskii and Wolff rearrangements (Arndt - Eistert synthesis), dienone - phenol (thermal and photochemical) -1 hour

Stevens, Somelet and Wittig rearrangements -1 hour

The benzidine rearrangement. Intramolecular migrations from nitrogen to carbon - the Orton, Fisher - Hepp and related rearrangements. Hoffman - Loffer Freytag reaction and Hauser rearrangement -2 hours

6. Free radical reactions:

Types of free radical reactions, free radical substitution mechanism, mechanism of an aromatic substrate, neighboring group assistance- -1 hour

Reactivity for aliphatic and aromatic substrates at a bridged head. Reactivity in the attacking radicals. The effect of radicals on reactivity -1 hour

Allylic halogenation (NBS), Oxidation of aldehydes to carboxylic acids. -1 hour

Auto oxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts -1 hour

Sandmeyer reaction. Free radical rearrangement. Hunsdiecker reaction -1 hour

McMurray Coupling, Barton Reaction, AIBN with (Bu)4Sn-H -1 hour

Diphenyl diselenide -1 hour

References:

Prescribed Books:

1. Michael B. Smith, March's, Advanced organic chemistry, 7th Ed., John Wiley & Sons, Inc, New York, 2016.
2. Carey and Sundberg, Advanced organic chemistry, 5th. Ed., Part B, Plenum Press, 2012.
3. J. Clayden, N. Greeves, S. Warren, Organic chemistry, 2nd Ed., Oxford University Press, 2012.
4. R.A.Y. Jones, Physical and Mechanistic Organic Chemistry, 2nd Ed., Cambridge University Press, 1984.
5. S. N. Mukherji, Pericyclic reactions, Macmillan, 1979.
6. P.S. Kalsi, Organic reactions and mechanisms, 3rd Ed., New Age International Publishers 2010.

Reference Books:

1. R.O.C Norman, J. M. Coxon, Principles of organic syntheses: 3rd Ed., CRC Press 1993.
2. H. Maskill, The physical basis of organic chemistry: Oxford science publications, 1985.

PCHM-205: Practical: Inorganic Chemistry

2 CREDITS

Course Objectives:

1. To perform semi-micro qualitative inorganic analysis of mixtures containing rare elements.
2. To prepare nanoparticles and characterize them.
3. To prepare quantum dots.

Course Outcomes: Upon completion, the student will be able to

1. Detect cations and anions in mixtures containing rare elements.
2. Prepare and characterize nanoparticles.
3. Perform water analysis using the techniques covered.

Syllabus:

Qualitative Analysis

1. Qualitative analysis of mixture of compounds containing rare elements such as Ti, V, Mo, W, Zr, Ce, U

Preparations

2. Synthesis and purification of Acetyl Ferrocene
3. Synthesis of Tetra Phenyl Porphyrin (TPP)
4. Spectrophotometric estimation of Ni/Cu/Zn by complexing with Tetra Phenyl Porphyrin (TPP)
5. Synthesis of HKUST-1
6. Synthesis of cis- and trans- Copper Glycinato Complexes
7. Preparation of manganese complex with acetylacetone (acac) and its applications in analysis

Nanoscience

8. Synthesis and characterization of carbon dots from organic waste
9. Synthesis of silver nanoparticles using aqueous floral petal extract

Water Analysis

10. Synthesis of water-soluble Alizarin Red S–Al(III) complex for fluoride ion sensing
11. Water quality monitoring using Ion Chromatography

Note: Minimum of 8 experiments need to be carried out.

References:

1. O. P. Vermani& A. K. Narula, Applied Chemistry (Theory & Practice), Wiley Eastern, 1989.
2. Vogel's Text Book of Macro and Semimicro Qualitative Inorganic Analysis 7thEd G. Svehla Orient Longman 2009.
3. N. K. Udaya Prakash et al., *Asian Journal of Chemistry; Vol. 27, No. 11 (2015), 4089-4091*
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PCHM-206: Practical: Physical Chemistry (Spectroscopy, Kinetics and Electrochemistry)
2 CREDITS
Course Objectives:
1. To learn physical chemistry principles using experiments. 2. To learn to prepare nanoparticles and study their growth kinetics. 3. To apply the elementary laws of chemical kinetics in the analysis of reaction mechanisms and understand the changes in chemical reactions. 4. To perform fluorescence-based experiments and learn to use a fluorimeter. 5. To learn to work with enzymes and also acquire the ability to study the kinetics of reactions involving enzymes. 6. To learn different electroanalytical techniques using the electrochemical workstation.
Course Outcomes: Upon completion, the student will be able to
1. Understand the principles behind the physical chemistry experiments performed and be in a position to explain them. 2. Prepare nanoparticles and also understand the growth kinetics. 3. Measure various kinetic parameters in different chemical systems and solve problems based on rate/rate constants for different types of reactions. 4. Perform fluorescence-based experiments and be able to operate a fluorimeter. 5. Design electrochemistry-based experiments and interpret the results by explaining the principles.
Syllabus:

1. **Excited state acidity constant measurement:** Determination of excited-state acidity constant of 2-Naphthol or any other fluorescent ionizable molecule
2. **Fluorescence quenching experiment:** Determination of rate constant for fluorescence quenching of Alq_3 (or any other fluorophore) by acrylamide, urea, Br- and I-
3. **Thermodynamics experiment:** Determination of enthalpy and entropy of excimer formation (e.g. pyrene or some other appropriate fluorophore)
4. **Kinetic salt effect:** To study the kinetics of reduction of Maxilon Blue-SG by sulfide Ion
5. **Nanoparticle growth kinetics:** Study of nanoparticle growth kinetics in zinc oxide using UV-Visible spectroscopy
6. **Spectroscopy experiment:** Raman spectroscopic studies on CCl_4, $CHCl_3$, CH_2Cl_2, Cyclohexane, C_6H_6, Toluene etc
7. **Cyclic voltammetry experiment:** Synthesis and cyclic voltammetry of Vanadium(III)acetylacetonate
8. **Activation energy determination:** Study of the kinetics of ethylacetate hydrolysis by NaOH using conductance measurements and determination of the energy of activation of the reaction
9. **CMC determination using spectroscopy:** To determine the critical micelle concentration (CMC) of anionic and cationic surfactants using conductance measurements and to study the influence of temperature on CMC. Verification of so determined CMC values using UV-Visible absorbance studies
10. **Enzyme kinetics:** Study of enzyme kinetics: hydrolysis of esters by α-chymotrypsin and the Michaelis-Menten equation
11. **Surface area determination:** Determination of surface area of activated charcoal/silica gel/ZnO/Zeolite using BET adsorption isotherm

Note: Minimum of 8 experiments need to be carried out.

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3. A. M. Halpern, Experimental Physical Chemistry, 3rd Ed., W. H. Freeman, 2006.

PCHM-207: Practical: Organic Synthesis (multistep) and Spectral Analysis
2 CREDITS
Course Objectives:
1. To give hands-on experience in carrying out various types of organic reactions including addition, elimination, condensation and functional group protection.
Course Outcomes: Upon completion, the student will be able to
1. Gain the skills and expertise to design and carry out organic reactions and use them in multi-step organic synthesis.
Syllabus:
Multi-step preparations of organic compounds illustrating the preparative uses of reactions such as aldol condensation, Mannich reaction, enamine reaction, Claisen condensation etc., and rearrangements such as Claisen, Fries, Beckmann, Wolff etc., Design and synthesis of organic compounds possessing novel features. Experiments involving - enamine reactions, Robinson annulation, Wittig reaction and protection-deprotection sequence (use of cyclic acetals in the protection of carbonyl - use of ester in the protection of alcohols or phenols etc.) Use of polymer-supported organic synthesis (Silica supported reagents, alumina-supported reagents etc.) **List of Experiments:** To perform any four of the following reactions and also characterize the products with spectroscopic techniques such as UV, IR, NMR and MS. 1. Mannich reaction and Vilsmeier-Haack formylation of indole. 2. Chiral organocatalysis- proline catalysed synthesis of β-hydroxy carbonyl compounds-(IR) 3. Wittig reaction under phase transfer conditions- synthesis of trans-stilbene-NMR 4. Synthesis of trans-cyclohexane -1,2-diol from cyclohexanol-MS and NMR 5. Ketal protection and reduction of -COOEt in ethyl acetoacetate-IR. 6. Achiral and Chiral Reduction of ethyl acetoacetate-Optical rotation. 7. Synthesis of APIs (compounds of pharmaceutical importance) – any three: Dihydropyrimidine, Isoniazid, Propranolol, 6-Methyl uracil and 2-*p*-Methoxy phenyl benzimidazole.
References:
1. D. J Pasto, C.R.Johnson and M.J.Miller, Experimental technique in Organic Chemistry, Prentice Hall, 1992. 2. L. M. Harwood and C.J. Moody, Experimental Organic Chemistry: Principles and Practice, Blackwell Scientific Publications, 1989 3. L.F. Tietze and Th. Eicher, Reactions and Syntheses, University Science Books, California, 1989. 4. B. S. Furniss et al., Vogel's Textbook of Practical Organic Chemistry revised, 5th Ed., ELBS, 1989. 5. Process chemistry Lab-manual -NIPER-HYDERABAD.

PCHM-301: Organometallic Chemistry
(3 CREDITS – 42 Hours)
Course Objectives:
1. To understand the basics of organometallic chemistry. 2. To study the synthesis, structure, geometry, bonding and characterization of various transition metal complexes with ligands such as carbonyls, dinitrogen, nitrosyl, hydrocarbons etc. 3. To understand the preparative methods, mechanisms and reactivity of various organo-transition metal complexes. 4. To learn the applications of organometallics in various industrially important catalytic processes.
Course Outcomes: Upon completion, the student will be able to
1. Predict the shape/geometry, stability of a given organometallic complex. 2. Predict the metal-ligand stoichiometry in an organometallic complex. 3. Write down the mechanism of a given organometallic reaction. 4. Possess the knowledge of important organometallic catalysts used in industry along with their mechanism.
Syllabus:

1. Introduction:

Overview of organometallics -1 hour

Organometallic chemistry definition and overview; Types of Ligands-L, X, Z; Hard and soft ligands; Ligands binding through sigma bonds, pi bonds, sigma and pi bonds, pi acceptors -1 hour

Agostic interaction, isoelectronic organometallic complexes and ligands -1 hour

18-electron rule and its limitations-16 electron rule -1 hour

2. Metal Carbonyls of Transition Elements:

Preparation of metal carbonyls - Structures of metal carbonyls (mononuclear, binuclear, trinuclear, tetra nuclear and poly nuclear) -2 hours

Bonding features: semi-bridging CO groups (in cyclic sets, in unsymmetrical environments and caused by steric crowding), Side-on bonding of CO - oxygen to metal bond -1 hour

Vibrational spectra of metal carbonyls (detection of bridging of CO groups, molecular symmetry, bond angles, mixture of conformers, force constants) -2 hours

Reactions of metal carbonyls: CO substitution reactions, photochemical reactions, Nucleophilic and electrophilic attacks on CO, Insertion reactions: CO insertion into M - C and M-H bonds -2 hours

3. Complexes with Other Ligands

Structure and bonding in metal complexes with Phosphines (Tolman cone angle, Tolman electronic parameter, Tolman plot), CS, CSe -1 hour

NO (Enemark-Feltham Notation), NO_2, CN, RNC -1 hour

Dinitrogen, Dioxygen ligands -1 hour

Metal hydride complexes, σ- complexes, -1 hour

4. Clusters and Metal-Metal Bonds

Introduction -metal carbonyl clusters: Low nuclearity carbonyl (M_3 and M_4) clusters -1 hour

High nuclearity carbonyl clusters ($HNCC_s$) – Skeletal electron counting, Wade's rules -1 hour

Capping rules -1 hour

Mingo's rules (polyhedra condensation), Jemmis rules -1 hour
Hetero atoms in metal atom clusters (carbides and nitrides) -1 hour
Isoelectronic and Isolobal relationships -1 hour

5. Compounds with M-M multiple bonds: Major structural types - Quadrupole bonds in clusters, One-dimensional solids. 2 hours

6. Transition Metal Complexes of Hydrocarbons
Metal alkyls, carbenes, carbynes and carbides -1 hour
Nonaromatic alkene and alkyne complexes –Metal carbenes-Fisher and Schrock carbenes -2 hours
Allyl and pentadienyl complexes - Metallocenes: synthesis and structures of cyclopentadienyl compounds -1 hour
Arenes and other Alicyclic Ligands- stability of polyene and polyenyl complexes, Davies-Green-Mingos' Rule -1 hour

7. Reactions of Organometallic Complexes
Oxidative addition reactions: Concerted additions-SN^2 reactions and radical mechanisms -2 hours
Hydrogen addition and HX additions - Reductive elimination reactions
-Oxidative coupling-reductive cleavage -2 hours
Insertion reactions: CO insertion into M - C and M-H bonds - Cyclometalation reaction -2 hours

8. Physical Methods in Organometallic Chemistry -2 hours
NMR spectroscopy, IR spectroscopy and Crystallography

9. Catalysis by Organometallic Compounds:
Homogeneous catalysts: Hydrogenation - Wilkinson's catalyst, Tolman's catalytic loops -1 hour
Hydroformylation (oxo process), Cativa process, Buchwald-Hartwig Reaction -1 hour
Synthesis gas, water gas shift reaction -1 hour
Olefin metathesis (Grubbs and Shrock's catalyst) -1 hour
Heterogeneous catalysts: Fischer-Tropsch process and Mobil process -1 hour
Ziegler-Natta polymerization, oligomerization -1 hour

References:

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1. R. H. Crabtree, The Organometallic Chemistry of the Transition Metals, 7th edition, 2019.
2. B. D. Gupta and A. J. Elias, Basic Organometallic Chemistry, 2nd Ed., University Press, 2015.
3. Gary L. Missler, Paul J. Fisher and Donald A. Tarr, Inorganic Chemistry, 5th Ed., Pearson, Delhi, 2014.
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9. B. Douglas, D. McDaniel and J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Ed; Wiley and Sons, New York, 1994.

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PCHM-302: Polymer Chemistry and Applications of Group Theory in Chemistry
(3 CREDITS – 42 Hours)
Course Objectives:
1. To study various methods employed in the synthesis of polymers and develop an understanding of the chemical kinetics and mechanistic aspects that are involved. 2. To understand the different types of molecular weights in polymers. 3. To derive selection rules for IR and Raman activity using group theory. 4. To construct molecular orbitals of metal complexes with ligands of different types. 5. To get free ion configurations terms and states, and Ligand Field Theory of coordination compounds. 6. To understand the origin of bands in the electronic spectra of coordination compounds.
Course Outcomes: Upon completion, the student will be able to
1. Design polymer synthesis schemes. 2. Assign the kinetic mechanism. 3. Compare compounds of different chemical behaviour under the same point group. 4. Draw molecular orbital diagrams of metal complexes. 5. Explain the spectra of coordination compounds and the origin of electronic transitions using Ligand Field theory.
Syllabus:
1. Step Polymerization: Mechanism of step polymerization - kinetics of step polymerization -1 hour Molecular weight control in linear polymerization -1 hour **2. Radical Chain Polymerization:** Nature of radical chain polymerization - Rate of radical chain polymerisation -1 hour Initiation - molecular weight - chain transfer - inhibition and retardation -1 hour **3. Emulsion polymerization:** Qualitative picture -1 hou **4. Ionic chain polymerization:** Comparison of radical and ionic polymerizations -1 hour kinetics - cationic polymerization of the carbon-carbon double bond -1 hour **5. Chain copolymerization:** Copolymer composition – Derivation of copolymer composition equation- ideal, alternate and block copolymers -1 hour **6. Ring-opening polymerization:** General characteristics - Cyclic ethers - Cyclic amides. -1 hour **7. Molecular weight:** Different types and their determination using end group analysis, membrane osmometry, light scattering, viscosity measurements and gel permeation chromatography -2 hours

Applications of Group theory:

8. **Molecular point groups:** Nonlinear-linear-cubic groups- Icosahedral point groups-notation of point groups-descent in symmetry in molecules with substitution -3 hours

9. **Symmetry criteria:** Symmetry condition for optical activity-symmetry restrictions on dipole moments and stereoisomerism. -1 hour

Normal mode analysis of non-linear molecules: Cartesian coordinate method, simple general method-Internal coordinate method (for molecules of different point groups). -2 hours

10. **Normal mode analysis for linear molecules:** Deductions of normal modes of vibrations for linear molecules: Integration method, Cyvin-Schafer method and Sub-group method -2 hours

11. **Infra-red and Raman spectroscopy of molecules:** Selection rules-IR and Raman activity-Symmetry requirements for overtones, binary and ternary combination bands, Fermi resonance. -2 hours

Crystal field splitting of d orbitals: Splitting of d-orbitals in transition metal complexes, Oh, Td, D4h -2 hours

12. **Molecular orbital theory of metal complexes:**

Molecular orbitals and hybrid orbitals and their symmetry species-hybrid orbitals for sigma, pi bonding-projection operation method and the ligand group orbitals -3 hours

MO theory of coordination compounds -2 hours

13. **Free ion configuration terms and states:**

Inter electronic repulsion parameters- spin orbit coupling parameters -2 hours

Symmetry of atomic orbitals and the spectral terms and correlation tables- -2 hours

Molecular term symbols: Derivation notation and selection rules for transition -2 hours

14. **Ligand Field Theory and Electronic Spectra of Metal Complexes**

Ligand field theory of coordination compounds: Simple crystal field theory of ML_6 complexes, effect of weak crystal field on terms, ligand field term diagrams, -2 hours

Expected electronic transitions-term interactions and the energies of levels-correlation diagrams -3 hours

Electronic spectra of metal complexes: Selection rules for electronic spectra-electric dipole transitions, magnetic dipole transitions -1 hour

nature of electronic spectral bands: Einstein coefficients, Band intensities (Relationship of transition moment integral with molar extinction coefficient and oscillator strength)-Bandwidths -2 hours

References:

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1. G. Odian, Principles of Polymerisation, 4th Ed., John Wiley & Sons., New Jersey, (2004).
2. F. W. Billmeyer, Jr., Text Book of Polymer Science, 3rd ed., John Wiley & Sons, New York (1984).
3. W. D. Callister Jr. and D. G. Rethwisch, Materials Science and Engineering – An Introduction, 9thEd., (2014), Wiley NJ.
4. Joel R Friend, Polymer Science and Technology, 3rd Ed., Pearson Education, New Jersey, (2014).
5. K. Veera Reddy, Symmetry and Spectroscopy of Molecules, New Age International (P) Ltd, Publishers 2ndrevised edition (2009).
6. A. B. P. Lever, Inorganic electron spectroscopy, 2nd Ed., Elsevier Amsterdam(1984)

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2. K J Laidler, and J H Meiser, Physical chemistry, Third Edition, Houghton Mifflin Company, Boston, New York (1999)
3. N B Colthup, LH Daly and S E Wiberley Introduction to Infrared and Raman spectroscopy, 2ndEd., Academic Press, New York (1975)
4. A. Streitweiser, Jr., Molecular Orbital Theory for Organic Chemists, John Wiley & Sons Inc., New York (1961)
5. Hargittai and M. Hargittai Symmetry through the Eyes of a Chemist, Verlagsgesellschaft, Germany(1986).
6. H H Jaffe and M Orchin Theory and Applications of UV spectroscopy, Wiley New York (1962).
7. M. Orchin, H H Jaffe, Symmetry Orbitals and Spectra, Symmetry orbitals and spectra, Wiley (inter science) New York (1970).

PCHM-303: Synthetic Organic Chemistry
(3 CREDITS – 42 Hours)
Course Objectives:
1. To introduce the following concepts in organic synthesis. i) Retrosynthetic approach. ii) Protection and deprotection of functional groups. iii) Solid support reagents and organometallic reagents. 2. To give an understanding of various types of organic reactions like: i) Oxidation and Reduction. ii) Asymmetric synthesis. iii) Photochemical reactions.
Course Outcomes: Upon completion, the student will be able to
1. Possess the knowledge of various aspects of organic synthesis such as retrosynthetic analysis, protection-deprotection of functional groups. 2. Gain good knowledge about various organic reactions and reagents used. 3. Design retrosynthetic analysis and propose a synthetic route for the synthesis of an organic compound.
Syllabus:

1. Synthetic Organic Chemistry - Concept and use of Protection & deprotection of sensitive functional groups in organic synthesis:

Alcohol -1 hour

Carbonyl - carboxyl -1 hour

Amine –lactone and thiols- problem solving -1 hour

2. Newer Synthetic Reagents - Polymer supported reagents and their applications in Peptide synthesis -1 hour

Solution phase synthesis versus solid supported synthesis -1 hour

Sheppard synthesis of peptides. -1 hour

Introduction to reactions on inorganic solid supports – Alumina -1 hour

Silica & zeolites -1 hour

Introduction to combinatorial Synthesis-Library synthesis on resin beads (only solid phase) -1 hour

3. Named Reactions:

Eschenmoser fragmentation, Nef reaction, Bamford Stevens reaction, Peterson Olefination reaction, Julia Olefination reaction, Nazarov Cyclization, Sharpless asymmetric dihydroxylation, Mitsunobu Reaction (Diethyl azodicarboxylate-DEAD), Fukyamaya-Mitsunobu reaction, C-H activation, N-heterocyclic carbene reactions.

-4 hours

4. Reductions in Organic Synthesis:

Hydroboration and its applications -1 hour

Metal / liquid ammonia reactions (Birch and related reductions) - catalytic reductions (Pd, Pt, Ni and Wilkinson's catalyst) - Catalytic transfer hydrogenation – Problem-solving -2 hours

5. Oxidations in Organic Synthesis – Alcohol Oxidations -1 hour

Alkene oxidations (Sharpless and other epoxidations), Prevost, Woodward and other hydroxylations -2 hours

Reactions with DDQ, Chloranil, Fenton's reagent and MnO_2
Swern's oxidation, Dess martin periodinane oxidation -2 hours

6. Planning a Synthesis - the basis for retrosynthetic analysis. -1 hour
Disconnections of C–C-, synthons, chirons, transform based strategies -1 hour
Strategic bond approach- with suitable example –cis-Jasmone – Problem solving -1 hour

7. Diastereoselectivity- Stereoselective reactions – Prochirality - Diastereoselective addition to carbonyl group without rings -2 hours

8. Asymmetric Synthesis: Chirality- chiral pool- resolution of enantiomers -1 hour
Chiral auxiliaries - alkylation of enolates -2 hours
Enantiomeric excess - asymmetric formation of c-c bonds-asymmetric conjugate addition - organocatalysis -2 hours

9. Electro-organic Syntheses
Electrode reactions classified by reaction type -1 hour

10. Organic Photochemistry
Alkenes: Isomerization, cycloaddition, di-Π methane reaction, ring closure -1 hour
Carbonyl compounds: Norrish type I & II reactions -2 hours
Aromatic photochemistry: Isomerizations, photoaddition, cycloadditions to the aromatic ring, singlet oxygen oxidations -2 hours

11. Organometallic Reagents in Synthetic Chemistry
Palladium catalysed vinylic substitutions- Stille coupling reactions, Suzuki coupling and Buchward-Hartwig reaction -2 hours

12. Total Synthesis of selected Natural Products – Reserpine -2 hours
Gilvocarcin-M -1 hour

References:

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1. J. Clayden, N. Greeves, S. Warren, Organic chemistry, 2nd Ed., Oxford University Press, 2012.
2. F. Carey and R.J. Sundberg, Advanced organic chemistry, 5th. Ed., Part B, Plenum Press, 2012.
3. Jie Jack Li, Name Reactions, 2nd Ed., Springer,2003.
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6. Laszlo Kurti and Barbara Czako, Strategic applications of Named reactions in organic synthesis, Elsevier, 2005.
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9. Ed. J.D.Coyle, Photochemistry in Organic Synthesis, RSC, 1986.
10. R.O.C Norman, J. M. Coxon, Principles of organic syntheses: 3rd Ed., CRC Press 1993.
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1. S. Warren, Designing organic synthesis, John Wiley Sons 1982.
2. E.J. Corey and Xue-Min Cheng, The Logic of Chemical Synthesis, John Wiley and Sons, 1995.
3. Albert J. Fry, Synthetic Organic Electrochemistry, 2nd Ed., John Wiley and Sons, 1989.
4. Jan Kopecky, Organic Photochemistry, VCH, 1991.

PCHM-304: Theory and Applications of Physical Methods in Chemistry
(3 CREDITS – 42 Hours)
Course Objectives:
1. To deliver in-depth knowledge of different spectroscopic techniques in elucidating the structure of various organic/ inorganic molecules and also to draw attention to the underlying principles involved.
Course Outcomes: Upon completion, the student will be able to
1. Interpret the given spectral data and elucidate the structure of the compound. 2. Deduce the chemical structure analyzing the spectral data. 3. Sketch the spectra of a given compound.
Syllabus:

1. Introduction: Selection rules for absorption of radiation by molecular vibrations, Intensity and line width of spectral lines. Population of various states and intensity. Doppler broadening and lifetime broadening, factors affecting coupling and degeneracy. -2 hours

Applications in Inorganic Chemistry

2. Infrared Spectroscopy: Vibrations of polyatomic molecules- fundamental vibrations and their symmetry- overtone and combination frequencies- Fermi resonance- -1 hour

The influence of rotation on the spectra of linear (polyatomic) molecules -1 hour

Effect of coordination on spectra due to change in symmetry – -1 hour

3. Microwave Spectroscopy:

Rotation of molecules and rotational spectra - Diatomic molecules - the rigid rotor -2 hours

intensity of spectral lines - effect of isotopic substitution- -1 hour

Non-rigid rotator, spectrum of non-rigid rotator - polyatomic molecules - linear, symmetric top and asymmetric top molecules (only spectral features) – -2 hours

Basic outline of the instrumentation of microwave technique. -1 hour

4. Raman Spectroscopy:

Raman scattering - theory of Raman effect - pure rotational Raman spectra of linear, spherical, symmetric top and asymmetric top molecules -2 hours

Raman activity of vibrations - Structure determination of CO_2, N_2O, SO_2, NO_3^-, ClO_3^- and ClF_3 using Raman spectroscopy -1 hour

Basic instrumentation -1 hour

5. Applications of NMR Spectroscopy in inorganic chemistry with special reference to ^{31}P, ^{19}F, ^{11}B nuclei -2 hours

and NQR spectroscopy -1 hour

6. Electron Paramagnetic Resonance:

Theory and applications to Nickel (II) & Copper (II) compounds, magnetic exchange process in dinuclear complexes -2 hours

7. Mossbauer Spectroscopy:

Origin and interpretation of Mossbauer effect, Mossbauer chemical shifts, Application of Mossbauer spectroscopy to Fe and Sn systems. -1 hour

Applications in Organic Chemistry and Biochemistry

8. Use of Shift Reagents – in U.V. Spectral Analysis, with examples chosen from the chemistry of naturally occurring flavonoids- where such methods have been particularly successful. -1 hour

9. I.R. Spectra with regards to the study of hydrogen bonding and resonance effects in organic compounds. -1 hour

10. Advanced Aspects of NMR:

NOE effect, FT NMR its advantage- -1 hour
AMX and Allylic systems, Coupling in substituted benzene rings -1 hour
Simplifying complex NMR spectra (second order spectra)-
High field instruments, Use of paramagnetic shift reagents. -1 hour
Double resonance, with particular reference to spin-spin decoupling -1 hour
Solvent effects in PMR spectra -1 hour
Protons on Oxygen, and Nitrogen
Heteronuclear coupling -1 hour
13C NMR – Introduction and Theory, Applications. -2 hours

11. Mass Spectrometry: High resolution mass spectral fragmentation mechanism, soft ionization techniques (CI, ESI, MALDI, FAB etc.) -1 hour

12. Combined Problem SolvingUsing UV, IR, NMR, Mass: Extensive analysis of problems based on integrated spectral data(UV, IR, NMR and MS). -3 hours

13. Two-dimensional NMR Spectroscopy:

Introduction - Theory and applications of DEPT spectra and Homo COSY -2 hours
Applications of Hetero COSY- HMQC and HSQC -2 hours
Incredible natural abundance double quantum transfer experiment (2-D INADEQUATE),
Introduction to and applications of NOESY
Problem solving -3 hours

References:

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1. Pavia, Lampman, Kriz and Vyvyan, Spectroscopy, Brooks/Cole, 2014.
2. Silverstein, Bassler and Morrill, Spectrometric Identification of Organic Compounds, 6th Ed., Wiley, 2013.
3. Horst Friebolin, Basic One and Two-Dimensional NMR Spectroscopy, 5th Ed. Wiley-VCH, 2011.
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6. E.A.V. Ebsworth, Structural Methods in Inorganic chemistry, 2nd Ed., D.W.H. Rankin and S. Cradock, 1991.

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2. J.W. Akitt, B. E. Mann, NMR and Chemistry, 4thEd., CRC Press,2000.
3. Nakanishi and Solomon, IR Spectroscopy, 2nd Ed, Holden Day 1977.

PCHM-305: Computational Applications in Chemistry – I
2 CREDITS
Course Objectives:
1. To expose the students to the basics of computer programming with Python. 2. To teach the quantum mechanical aspects of molecular modelling. 3. To use computational software for the calculation of various properties.
Course Outcomes: Upon completion, the student will be able to
1. Write basic programs in Python. 2. Perform computational calculations on molecules. 3. Calculate various properties using computational software.
Syllabus:

Familiarity with Chemical Structure Drawing Software -3 hours
Plotting and Data Fitting -3 hours
Linux, DOS Commands -6 hours

Computer Programming - Python -42 hours
Drawing Flow charts
Introduction to Python: Using Python Shell, Running Python Scripts, Introduction to Idle, Errors in Python and their Types, Rules for Identifiers and Python Reserved Words
Data Types: Numeric and Non-Numeric Types – Integers and types, Strings – Concatenation, Slicing, Important String Functions; Float, Complex Type, Bool; Type Conversion
Variables: Immutable and Mutable, Memory Management; Comments; Constants;
Operators: Types of Operators, Arithmetic Operators, Relational Operators, Logical Operators, Assignment Operators and Types, Compound Operators, Identity Operators, Membership Operators, Precedence and Associativity of Operators, Is Operator
Decision Control Statements: If Statement, If-Else Statement, If-Elif-Else, Ternary Operator
Iterative Statements: Loops and Types-While Loop, While-Else Loop with Break, Continue and Pass Statements; For Loop with and without Range function;
Functions: Print()-Singleline, Multiline with Special Characters; Input() – Accepting Single/Multiple Value(s), Id Function, Eval( ) Function, Command Line Arguments and Various Print( ) Options; Function V/s Method, User Defined Functions - Calling a Function, Returning Values from Function

Electronic Structure Analysis -27 hours
1. Overview of the Software
2. Construction of z-matrix
3. Energy Minimization/Geometry Optimization, Single Point Energy Calculation
4. Molecular Mechanics, Semi-empirical, Ab-Initio and DFT Calculations
5. Introduction to Basis Sets
6. Modelling Transition State
7. Molecular Orbital Calculations and Visualization
8. Obtaining Electronic Spectra of organic molecules

Data Science and Data Mining in Material Science -3 hours

References:

1. David Amos, Dan Bader, Joanna Jablonski, Fletcher Heisler, Python Basics: A Practical Introduction to Python3, 4th Ed., Real Python (Realpython.Com), ISBN-13:978-1775093329, 2021.
2. Brian Heinold, A Practical Introduction to Python Programming, BrianHeinold.net (2015) Prentice Hall. 2015
3. K. I. Ramachandran, G. Deepa, K. Namboori, Computational Chemistry and Molecular Modelling Principles and Applications Springer-Verlag Berlin Heidelberg, ISBN-13 978-3-540-77302-3. 2008.
4. Errol Lewars, Computational Chemistry Introduction to the Theory and Applications of Molecular and Quantum Mechanics 3rd Ed., 2004 Kluwer Academic Publishers New York, Boston, Dordrecht, London, Moscow, ISBN: 1-4020-7285-6. 2018.
5. David C. Young, Computational Chemistry: A Practical Guide for Applying Techniques to Real-World Problems. John Wiley & Sons, Inc. 2011.
6. C. J. Cramer, Essentials of Computational Chemistry Theories and Models, 2004 ISBN 0-470-09182-7

PCHM-306: Project work (Interim Review)
Course Objectives:
1. To train the students in doing a scientific literature review/survey based on a field/topic chosen by them: Reading & collating the summaries of the important research papers in the field. 2. To identify the gaps in existing knowledge in the chosen topic based on the literature review and define the objectives for the project accordingly. 3. To understand the different possible experimental designs. 4. Charting down feasible and achievable work plans to accomplish the proposed objectives.
Course Outcomes: Upon completion, the student will be able to
1. Do a scientific literature review. 2. Identify gaps in the existing research and phrase potential objectives for a project. 3. Plan a few probable experimental designs to achieve the identified objectives.
Interim Review Assessment: At the end of the third semester, the assessment of the project work will be done based on the objectives of the problem identified by the student, the depth of literature review done and the proposed work plan for achieving the objectives.

PCHM-401: Solid State Chemistry and Nanomaterials
(2 CREDITS – 28 Hours)
Course Objectives:
1. This unique course emphasises on solid-state materials and their properties. 2. To introduce the concepts underlying solid state chemistry. 3. To synthesize and characterize a wide range of solid state materials and study their properties. 4. To offer an overview of carbon nanomaterials and their synthesis.
Course Outcomes: Upon completion, the student will be able to
1. Have knowledge of different methods used in the preparation of solid-state materials and their properties. 2. Give the principle of XRD technique and its use in crystal structure determination. 3. Understand the various methods to prepare carbon nanomaterials and give their applications.
Syllabus:

1. Preparative Methods:

Solid state reactions general principles, experimental procedure, -1 hour
Co-precipitation as a precursor to solid state reactions, -1 hour
Kinetics of solid state reactions -1 hour
Crystallizations of solutions, melts, glasses and gels, vapour phase transport methods, ion exchange reactions, electrochemical reduction methods and thin film preparation, growth of single crystals -2 hours

2. X-Ray Diffraction:

X-rays and their generation-an optical grating and diffraction of light, crystals and diffraction of x-rays -2 hours
X-ray diffraction experiment, the powder method-principles and uses, single crystal methods-principle and uses -2 hours
High temperature X-ray diffraction, electron diffraction and neutron diffraction -2 hours

3. Electronic Properties and Band Theory:

Introduction- metals, insulators and semiconductors -1 hour
Electronic structure of solids- band theory -1 hour
Colour in inorganic solids. -1 hour

4. Electrical Properties:

Hall effect, dielectric materials, ferro-pyro-piezo electricity and its applications -1 hour

5. Magnetic Properties: Classification of materials -Dia, para, ferro, ferri, and antiferromagnetic types -2 hours
Selected magnetic materials such as spinels, garnets and perovskites -1 hour

6. Superconductivity: Theory, discovery and recent high Tc materials -2 hours

7. Organic Solids State Chemistry:

Topochemical control of organic solid-state reactions
Electrically conducting solids, organic charge transfer complex, organic metals, new superconductors -2 hours

8. Carbon Nanomaterials:

Synthesis of Nanomaterials: Top down and bottom up synthesis approach, physical and chemical techniques for nanomaterial synthesis -2 hours
Sol-gel and hydrothermal methods -1 hour
Carbon Nanotubes and carbon clusters -2 hours
Applications of carbon nanotubes -1 hour

References:

PRESCRIBED BOOKS:

1. A. R. West, Solid State Chemistry and its Applications (Student Edition), W. S. E. Wiley, 2014.
2. Poole and Owens, Introduction to Nanotechnology Wiley, 2020.
3. L. Smart and E. Moore, Solid State Chemistry, Chapman Hall 1992.

REFERENCE BOOKS:

1. Geoffrey A Ozin, André C Arsenault, Nanochemistry: A Chemical Approach to Nanomaterials. Royal Society of Chemistry, 2005.
2. L.V. Azaroff, Introduction to Solids. Tata Mcgraw Hill, 1977.
3. A. R. West, Solid State Chemistry and its Applications, W. S. E. Wiley, 2003.

PCHM-402: Supramolecular Chemistry

(2 CREDITS – 28 Hours)

Course Objectives:

1. To teach concepts central to non-covalent interactions and host-guest interactions.
2. To give an understanding of supramolecular self-assembly in biological and synthetic systems.

Course Outcomes: Upon completion, the student will be able to

1. Appreciate the role of interactions in supramolecular assemblies and their applications in organic chemistry, chemical biology, materials science and nanotechnology.
2. Design functional materials with desired properties by exploiting non-covalent interactions, molecular recognition and self-assembly.

Syllabus:

1. Non-covalent Interactions: -5 hours

Electrostatic interactions (Ion pairing, Ion-Dipole interactions, Dipole-Dipole interactions, Dipole-Induced Dipole and Ion-Induced Dipole interactions, van der Waals, London-Dispersion forces), Solvophobic interactions, Hydrogen bonding, Halogen bonding, Cation-π interactions, Anion-π interactions, π - π interactions, Aromatic-Aromatic Interactions: Edge-to-face vs. π-π Stacking Interactions, Benzene-Hexafluorobenzene π-stacking, Composite interactions: N-H- π, C-H-π, interactions; Electron transfer interactions: n□π* and charge□π* interactions; Chalcogen bonds.

2. Concepts Central to Molecular Recognition: -5 hours

Host-Guest Chemistry; Macrocycles, clefts and open chain host structures; Receptors, Coordination and the "Lock and Key" analogy; Chelate, Macrocyclic and Cryptand effects; Pre-organization and Complementarity; Thermodynamic and Kinetic Selectivity; cooperativity and multi-valency.

3. Receptors: -5 hours

Cation Binding Hosts: Podands, Crown Ether, Cryptands, Spherands, Calixarenes and Siderophores; Anion binding hosts; Hosts for Neutral Receptors - Clathrates, Inclusion Compounds, Zeolites, Intercalates, Coordination Polymers, Guest Binding by Cavitands and Cyclodextrins, Cucurbituril.

4. Supramolecular Aspects of Chemical Biology: -5 hours

Molecular recognition, Supramolecular assembly of DNA, Supramolecular reactivity and catalysis, Multisite recognition.

5. Self-Assembly and Supramolecular Devices: -5 hours

Self-assembly, and applications to Catenanes, Rotaxanes, Helicates, gels, and molecular machines; Principles and applications of nanobiotechnology; Transporters and Carriers design.

6. Metal-Organic Framework Materials: -3 hours

Synthesis, properties, and applications in storage and separation of strategically important gases (H_2, CO_2, CH_4), drug delivery, and energy.

References: -
Prescribed books: 1. J. W. Steed, J. L. Atwood. Supramolecular Chemistry. John Wiley and Sons, 2000. 2. J. -M. Lehn, Supramolecular Chemistry. Concepts and Perspectives. VCH, 1995. 3. H.-J. Schneider, A. Yatsimirsky. Principles and Methods in Supramolecular Chemistry. John Wiley and Sons. 2000. **Reference books:** 1. J. N. Israelachvilli. Intermolecular and Surface Forces, 3rd ed., Academic Press, 2011.

PCHM-403: Medicinal Chemistry

(2 CREDITS – 28 Hours)

Course Objectives:

1. To give an outline of the process of drug design and the basic aspects related to it.
2. To give an overview of the synthesis and action of water-soluble vitamins and a few classes of antibiotics.
3. To give an idea about the utility of natural products as leads for new pharmaceuticals with special reference to medicinal plants of Indian and Chinese origin.
4. To understand the basic aspects related to drug molecules.

Course Outcomes: Upon completion, the student will be able to

1. Gain knowledge about the entire process involved in drug design and discovery from lead molecule to a drug.
2. Predict the metabolism of drugs.
3. Understand the structure-activity relationship of a few antibiotics.
4. Appreciate the use of natural products as drug candidates.

Syllabus:

1. Drug Design:

The drug discovery process - conceptual back-ground - Drug receptors	-2 hours
Drug target binding forces	-1 hour
History and development of QSAR	-1 hour
Effect of physical properties of the drug on its action (Ferguson and related theories)	-2 hours
Concept of lead structure & pharmacophore – Concept of isosterism and bioisosterism	-2 hours
Three-dimensional structure - aided drug design (use of relevant software to get hands on experience)	-1 hour

2. Pharmacokinetics & Pharmacodynamics:

Introduction of drug absorption, bioavailability (factors affecting and dosage determination)	-2 hours
and metabolism -Phase I & Phase II	-2 hours

3. A Study of Antibiotics:

Chemistry and pharmacology of streptomycin	-2 hours
Structure and Pharmacology of tetracyclines (detailed structure elucidation of tetracycline)	-2 hours
Gramicidin, a survey of anticancer antibiotics	-1 hour

4. Dietary Factors:

Study of water-soluble vitamins (Structure elucidation, synthesis)	
Chemistry and biological functions of Thiamine	-2 hours
Riboflavin	-1 hour
Pyridoxine	-1 hour
Pantothenic acid and Folic acid	-2 hours

5. Drugs from Medicinal Plants:

A study of active ingredients of some well-established Indian medicinal plants	-2 hours
A survey of Chinese medicinal plants	-2 hours

References:
PRESCRIBED BOOKS: 1. Foye's Principles of Medicinal Chemistry, Thomas Lemke and other editors, Lippincott Williams & Wilkins; 7th Ed., 2012 2. M. E. Wolff, (Editor) Burger's Medicinal chemistry, Volume I, 5th Ed, John Wiley & Sons, 1995. 3. Thomas L Lemke, Victoria F Roche, S William Zito, David A. Williams,Foye's Principles of Medicinal Chemistry (South Asian Edition) 8th Ed. Wolters Kluwer (Publisher),2020 4. C. Hansch, P.G. Sammes and J. B. Taylor(Editors) Comprehensive Medicinal Chemistry Vols 1 and 4, Pergamon Press, 1990. 5. Molecular Recognition of Amiloride Analogs: A Molecular Electrostatic Potential Analysis, J. Med. Chem., 35, p 1643, 1992. 6. Robert K. Murry, D.K. Granner, P.A. Mayes and V.W. Rodwell Harper's Biochemistry,25th Ed. McGraw Hill, Lange medical books,1999 **REFERENCE BOOKS:** 1. J.B. Taylor and P.D. Kennewell, Introductory Medicinal Chemistry, Ellis Horwood, 1981. 2. Yvonne Connloy Martin, Eber Hard Kutter, VolkhardSustel(Editors), Modern Drug Research, Vol.12, Paths to better and safer drugs, Marcel Dekker. Inc, 1989.

PCHM-404 E-I (i): Environmental Chemistry
(Elective) (3 CREDITS – 42 Hours)
Course Objectives:
1. Demonstrate knowledge of chemical and biochemical principles of fundamental environmental processes in air, water, and soil. 2. Recognize different types of toxic substances & responses and analyze toxicological information. 3. Apply basic chemical concepts to analyze chemical processes involved in different environmental problems (air, water & soil). 4. To create awareness about various water purification methods, wastewater treatment methods and the chemistry involved. 5. To study the cause and effect of environmental pollution by hazardous wastes and some mitigation strategies. 6. To explain the present energy crisis and different aspects of sustainability. 7. To understand the role of ethical values in addressing environmental issues.
Course Outcomes: Upon completion, the student will be able to
1. Use technical and analytical skills to quantify the level and effects of xenobiotics in environmental compartments (air, water, soil, biota). 2. Apply the concepts studied in the course to solve environmental problems. 3. Understand the need to live in harmony with nature.
Syllabus:

1. Air Pollution:

Air pollutants - Air quality standards -1 hour

Production, fate, effects and control of gaseous pollutants - Oxides of carbon, nitrogen and Sulphur - Organic air pollutants -1 hour

Photochemical reactions, photochemical smog, Greenhouse effect 2 hours

Acid rain and Ozone depletion. -1 hours

Particles in the atmosphere - physical behaviour - physical and chemical processes for particle formation -1 hours

Composition of inorganic and organic particles- toxic metals and radioactive particles Effects and control of particles -1 hour

2. Water Pollution:

Water quality - Water pollutants (inorganic and organic) - Sources, fate, effects and controlling measures - Chemical speciation -2 hours

Pollution by Radionuclides - Biochemical oxygen demand-Chemical oxygen demand, -2 hours

Eutrophication, Biodegradation of pollutants. -1 hour

3. Water Treatment:

Hardness of water and its removal - removal of solids and other toxic materials -1 hour

Treatment of water for drinking - Electrodialysis, ion exchange, -1 hour

Reverse osmosis, desalination processes, -1 hour

Removal of iron, manganese, phosphorous, calcium and nitrogen -1 hour

Treatment of water for industrial purposes – -1 hour

Sedimentation, coagulation, flocculation, filtration,	-2 hours
Adsorption, disinfection of water –	-1 hour
Sewage treatment (physical and chemical methods) –	-1 hour
Health effects of drinking water treatment technologies	
Impact of detergents, pesticides and other additives on sewage treatment.	-1 hour
4. Oils in Fresh & Marine Water:	
Sources of oil pollution -Chemistry and fate of hydrocarbons	
Oil in runoff and groundwater –	-1 hour
Biodegradation - effect on aquatic organisms and commhouries –	-1 hour
Treatment and disposal technology.	-1 hour
5. Soil Pollution:	
Soil pollutants -Inorganic, organic	
Pesticides, radionuclides	-1 hour
Sources and effects on nature and properties of soil, crops, plants and terrestrial animals.	-1 hour
6. Hazardous Wastes:	
Nature and sources of hazardous wastes	-1 hour
Classification, characteristics & constituents	-1 hour
Transport and effects	-1 hour
Hazardous wastes in Geosphere, Hydrosphere, Biosphere and Atmosphere	-2 hours
Reduction, treatment by physical and chemical methods	-1 hour
Thermal treatment methods	-1 hour
Biodegradation of wastes	-1 hour
Disposal of hazardous wastes. Waste management and Industrial by-products	-1 hour
Natural hazards and management- control of subsurface migration of Hazardous Waste	-1 hour
E-Waste: effect on the environment: Sources-constituents and their effects-pollution of water, soil and air-Methods of treatment and disposal-Extraction of gold and other precious metals from E-waste.	-3 hours
7. Values in Environment:	
The philosophy and Technology of living in tune with nature and its assets	-1 hour
Nature-A silent teacher, Ecology-The Indian Approach	-1 hour

References:

PRESCRIBED BOOKS:

1. Stanley E. Manahan, Environmental Chemistry .10th Ed., CRC Press, 2017.
2. Vander Meulen and Hrudey, Oil in FreshWater, Pergamon, 1987.
3. Lippmann and Schlesinger, Chemical Contamination in the Human Environment, OUP, Oxford, 1979.
4. John C. Crittenden, R. Rhodes Trussell, David W. Hand, Kerry J. Howe, George Tchobanoglous, Water Treatment - Principles and Design, 3rd Ed., Wiley, 2012.

REFERENCE BOOKS:

1. B.J. Finlayson– Pits and N.N. Pitts Jr., Atmospheric Chemistry, Wiley, 1986.
2. M.M. Varma, Hazardous and Industrial Wastes, HMCRI, 1988.
3. J.M. Montgomery, Water Treatment - Principles and Design, Wiley, 1985.

PCHM-404 E-I (ii): Functional Materials
(Elective) (3 CREDITS-42 hours)

Course Objectives:

1. Overview of materials used in various functional devices.
2. Understand the working of various functional devices using these materials.
3. Teach the structure, composition and role of various materials used in functional devices.

Course Outcomes: Upon completion, the student will be able to

1. Gain knowledge of different kinds of materials used in functional devices.
2. Explain the working of various functional devices using these materials.
3. Know the structure, composition and role of various materials used in various functional devices.
4. Apply the knowledge gained in designing materials for the applications studied.

Syllabus:

1. Introduction to Materials, Classification with examples -2 hours

2. Introduction to Crystals:
Lattice, Unit Cell, Types of Lattices/ Bravais Lattice, Lattice Planes, Miller Indices
Defects and Types: Point, Linear, Planar, Volume -2 hours

3. Material Synthesis:
Soft Chemistry Routes -1 hour
Preparation of Materials in Different Configurations (Bulk, Polycrystalline, Ceramic, Single Crystals, Thin Films) -1 hour
Crystal Growth Techniques -2 hours
Thin Film Preparation: AC/DC Sputtering, Laser Ablation, Growth Kinetics
Influence of Substrate Material on the Growth Aspects of Films; -1 hour
Solid-State Reaction Route, Kinetics of Solid-State Reactions, Mechanical Alloying -1 hour

4. Characterization Techniques
X-ray/Electron/Neutron Diffraction -1 hour
SEM, CryoSEM, TEM, EDX -2 hours
X-PES (ESCA), UV-PES -1 hour
STM, AFM - Principle, Various Imaging Modes -1 hour
Concentration, Size and Zeta Potential Measurement by Light Scattering
Size determination by Absorption Spectroscopy -1 hour
TGA, DTA, DSCPrinciple, Working and Applications -1 hour
Characterization of Magnetic Materials: Susceptibility – Magnetic, Diamagnetic, Paramagnetic and their Measurement; Magnetism – Ferro, Ferri, Antiferro -1 hour

5. Organic Electronic Materials:

Basic theory and design of Molecular wires, Resistors, Diodes, Logic Gates	-2 hours
Organic Light Emitting Diodes: Introduction, Structure of OLEDs, Working, Applications	-1 hour
Fabrication methods, Types - OLEDs, PLEDs, Various Configurations	1 hour
Different Generations – 1st, 2nd, 3rd, 3.5th	-1 hour
p-type Materials, n-type Materials, Ambipolar materials	-1 hour
Materials for Blue/Green /Red/white OLEDs, Quantum Dot OLEDs, TADF Materials	-1 hour
Perovskites- Synthesis, Structure, Characterization, Electronic Properties and Applications	-2 hours

Transistors/OFETs -Structure, Various design configurations, Fabrication, Working and Applications Types of Molecules used and their properties -2 hours

Conducting/Semiconducting Materials: Small Molecules, Polymers: Types of Conducting Polymers. Chemical and Electrochemical Routes of Synthesis. Doping and Dedoping of Conjugated Polymers. Soliton, Polaron, Bipolaron Formation in Conducting Polymers. Conduction Mechanisms. -2 hours

6. Organic Photonic Materials:

Organic Solar Cells - Fabrication, Working Mechanism and Characterization, 1,2,3 Generations	-3 hours
Molecules for NLO and Imaging	-1 hour
Photorefractive Materials	-1 hour
Photoconductive Materials	-1 hour
Photochromic and Electrochromic Materials	-1 hour

7. Other Applications: Smart Materials, Thermoelectric Materials
Piezoelectric Materials, Pyroelectric Materials, Ferroelectric Materials -4 hours

References:

1. R J D Tilley, Understanding Solids: The Science of Materials, Wiley, 2013.
2. W. F. Hosford, Materials Science: An Intermediate Text, Cambridge Univ. Press, 2011.
3. James F. Shackelford, Introduction to Materials Science for Engineers, Prentice Hall, 2015.
4. Milton Ohring, Materials Science of Thin Films, II Edition, Academic Press 2001.
5. W. D. Callister, Materials Science and Engineering, Wiley, 2010.
6. Anthony R West, Solid State Chemistry and its Applications, Wiley, 2014.
7. Yang Leng, Materials Characterization: Introduction to Microscopic and Spectroscopic Methods, John Wiley & Sons (Asia) Pvt. Ltd., 2013.
8. Sam Zhang, Lin Li, Ashok Kumar, Materials Characterization Techniques, CRC Press 2009.
9. Douglas A. Skoog, F. James Holler, Stanley R. Crouch, Principles of Instrumental Analysis, 7th ed., Cengage Learning 2018.
10. T. J. J. Müller and U. H. F. Bunz, Functional Organic Materials Wiley-VCH, 2007.
11. Sam-Shajing Sun, Larry R. Dalton, Introduction to Organic Electronic and Optoelectronic Materials and Devices CRC Press, 2008.
12. S. Ogawa, Organic Electronics Materials and Devices Springer, 2015
13. Craig A. Rogers, Intelligent Materials –Scientific American, p. 122, 1995.
14. B. Culshaw, Smart Structures and Materials, Artech House, Norwood, MA. 1998.
15. Y. Osada and S.B. Ross – Murphy, Intelligent Gels Scientific American, May1993.

PCHM-404 E-1 (iii): Photophysics of Organic Molecules

(Elective) (3 CREDITS-42 hours)

Course Objectives:

1. To introduce the students to the new area of chemistry known as photophysical chemistry of organic molecules.
2. To make students aware of the intricacies of all the radiative and non-radiative events taking place in a molecule.
3. To make students understand the fundamentals, principles and instrumentation of ultrafast spectroscopic techniques.

Course Outcomes: Upon completion, the student will be able to

1. Understand photophysical chemistry and its nuances.
2. Possess the knowledge of all radiative and non-radiative processes happening in a molecule and be able to apply them to explain processes happening in a novel molecule.
3. Understand the fundamentals, principles and instrumentation of ultrafast spectroscopic techniques and be able to identify the best technique for a problem at hand.

Syllabus:

1. Basics:

Frank-Condon Principle, Oscillator Strength, Absorption Cross-Section, Extinction Coefficient, Einstein's A and B Coefficients, Fermi-Golden Rule, Types of Transitions – CT, MLCT, LLCT, MMCT, LMCT, TICT -3 hours

Instrumentation: Light Sources, Wavelength Selectors, Sample Holders and Detectors – Photodiodes, PMTs, CCDs -2 hours

2. Fluorescence Spectroscopy:

Luminescence, Types of Luminescence, Singlet State Vs Triplet State, Kasha's Rule, Absorption Spectra vs Fluorescence Spectra, Fluorescence vs Phosphorescence; Stokes Shift, Photobleaching, Self-Absorption; Fluorophores – Intrinsic, Extrinsic with examples -2 hours

Fluorescence Setup – L-Format, T-Format; Fluorescence Measurements – Steady State and Time Resolved Parameters Measured in Fluorescence Experiments -1 hour

Lifetime Measurements – Phase Fluorometry, Pulse Fluorometry (TCSPC) -3 hours

Variables That Affect Fluorescence & Phosphorescence Quantum Yield; Effect of Fluorophore Concentration on Fluorescence Intensity - derivation -2 hours

Solvent Effects – General and Specific; Solvent Relaxation, Fluorescence Quenching and its types -2 hours

Fluorescence Polarization, Fluorescence Anisotropy, Fluorescence Resonance Energy Transfer (FRET) -3 hours

Fluorescence Sensing; 2D Electronic Spectroscopy -2 hours

3. Photophysics of Organic Molecules:

Physical and Photophysical Processes in Electronically Excited Molecules; Radiative Transitions – Delayed Fluorescence (E-Type and P-Type) and Phosphorescence -1 hour

Spin-Forbidden Radiative Transitions and Spin-Orbit Coupling -1 hour

Radiative Transitions in Molecular Complexes, Excimers and Exciplexes, Emission from Excited Singlets and Triplets – Azulene Anomaly -1 hour

Non-Radiative Transitions – Parameterized Model of Radiationless Transitions, Relation of Rates and Efficiencies of Radiationless Transitions to Molecule Structure, Factors Influencing the Rate of Vibration Relaxation -2 hours

Evaluation of Rate Constants for Radiationless Processes, Internal Conversion (S_n-S_1), Intersystem Crossing (S_1-T_1, T_1-S_0), Perturbation of Spin-Forbidden Radiationless Transitions -2 hours

Electron Transfer: Markus Theory -2 hours

Proton-Coupled Electron Transfer, Redox Properties of Excited States of Coordination Compounds: The Case of $[Ru(Bpy)_3]^{2+}$ -1 hour

4. Ultrafast Spectroscopy:

Principle. Instrument layout, Working and Applications of Microsecond Spectroscopy, Nanosecond Spectroscopy, Picosecond Spectroscopy, Femtosecond Spectroscopy - Fluorescence Upconversion, Transient Absorption Spectroscopy, Attosecond Spectroscopy -6 hours

Degenerate Four-Wave Mixing (DWFM) – Principle, Instrument layout and Application of DFWM in Study of - Femtosecond Excited Dynamics, Rotational Dynamics and Solvation Dynamics -6 hours

References:

PRESCRIBED BOOKS

1. Rohatgi Mukherjee, Fundamentals of Photochemistry 3rd Ed., New Age International Publisher 2018.
2. Nicholas J. Turro, Modern Molecular Photochemistry University Science Books 1991.
3. John Betteley Birks, Photophysics of Aromatic Molecules, Wiley Interscience, London 1970.
4. A. H. Zewail, Femtochemistry : Ultrafast Dynamics of the Chemical Bond, World Scientific, 1984.
5. W. T. Silfvast, Laser Fundamentals, Cambridge. 2003.
6. H. Abramczyk, Introduction to Laser Spectroscopy, Elsevier 2005.
7. Atanu Bhattacharya, Ultrafast Optics and Spectroscopy in Physical Chemistry, World Scientific-IISc Press, 2017.

REFERENCE BOOKS

1. Skoog, Holler and Crouch, Principles of Instrumental Analysis, 7th Ed., Cengage Learning, 2017.
2. J. Michael Hollas, Modern Spectroscopy, 4 Ed., Wiley-Blackwell; 4th edition, 2003.
3. Gerhard Hertzberg, Molecular Spectra and Molecular Structure, Vol-I and II, Read Books Ltd, 2013.
4. Joseph R. Lakowicz, Principles of Fluorescence Spectroscopy 3rd Ed., Kluwer Academic/ Plenum Publishers, 1999.
5. Bernard Valeur and Mario N. Berberan-Santos, Molecular Fluorescence: Principles and Applications, 2nd Ed., Wiley-VCH, 2013.
6. A. Douhal, ed. Femtochemistry and Femtobiology: Ultrafast Dynamics in Molecular Science, World Scientific, 2002.

PCHM-405 E-II (i): Biocatalysis for Industry and Environment
(Elective) (3 CREDITS – 42 Hours)
Course Objectives:
1. To study the advantages and limitations of biocatalysts in organic synthesis and the criteria that one may choose for using biocatalysts over conventional catalysts. 2. To provide an overview of the different enzyme classes coupled to the catalyzed chemical reactions with stereochemistry involved and methods to optimize the stereochemical outcome. 3. To introduce the concept of bioreactors, various configurations and modes of operation. 4. To discuss several industrial bioprocesses such as biomass hydrolysis, enzymatic conversion of biomass components like cellulose, hemicellulose and lignin to sugars and other value-added products. 5. To learn about the large-scale bioremediation techniques employed towards remediating contaminated soils and water bodies for controlling pollution.
Course Outcomes: Upon completion, the student will be able to
1. Distinguish reaction mechanisms of enzymes from the different main classes and be able to choose preferred enzymes based on their class for the various chemical reactions. 2. Recognize advantages and disadvantages of different reaction media for enzymatic reactions and be able to decide suitable reaction conditions as per the individual reactions. 3. Decide and choose an appropriate bioreactor configuration needed based on the biotransformations to be carried out. 4. Appreciate the commercial importance of bioprocesses towards the production of value-added products in several industries. 5. Have the knowledge of the large scale bioremediation techniques employed in Environmental remediation and pollution control.
Syllabus:

1. Biotransformation, Biocatalyst and Chemical Industry:
Basic organic reaction mechanism, common prejudices against enzymes, advantages and disadvantages of biocatalysts, isolated enzyme versus whole cell systems, Enzymatic and Microbial Reactions -4 hours
Application in Organic Synthesis: Hydrolytic Reactions, Reductions, Oxidations, Formation of C-C Bonds. -2 hours
Additions and Eliminations Reactions. -2 hours
Special Techniques Involving the use of Enzymes and Microorganisms: Extending and Improving Bio-transformations, Purified Enzymes/ Crude Enzymes, Extracts, Substrate Modifications. -2 hours
Effects of Temperature on Enzyme Selectivity, Enzymes in Organic Solvents, Advantages of Biotransformations in Organic Solvents. -1 hour
Designing a Solvent System for Enzyme-Catalyzed Reactions. -1 hour
Immobilized Enzymes and Immobilized Microorganisms, Principal Immobilization techniques, Lipase powders. -2 hours
Enzymes Covalently Bonded on Neutral Polymers, Cross-Linked Enzyme Crystals (CLEC). Cofactor Regeneration Techniques- -1 hour

2. Microbial Kinetics Reaction theory and kinetics, Cell growth and kinetics. -1 hour
Yield and maintenance, coefficient concepts, Determination of microbial kinetics from batch data -1 hour

Substrate utilization and product formation kinetics. -1 hour
Enzyme inhibition, reversible inhibition, -1 hour
non-competitive/uncompetitive inhibition, irreversible inhibition. -2 hours
pH effects on enzyme kinetics. -1 hour

3. Bioreactor Operation
Batch, fed-batch and chemostat operation of bioreactors, Evaluation of kinetic and yield parameters in chemostat culture, Bioreactor configurations, Fermentor operation – initiation, operation and harvest of batches -2 hours
Application of Biotechnology to Chemical Production, Single-step Reactions of Commercial Importance, Multi-step Reactions of Commercial Importance -2 hours
Biomass hydrolysis, enzymatic conversion of biomass components (cellulose, hemicellulose and lignin) to sugars and other value-added products. Enzymes commonly used in processing systems: Carbohydrases, proteases, lipases and oxidoreductases. -2 hours
Biological Routes to Optically Active Epoxides, The Production of Optically Pure Natural and Unnatural Amino Acids, hydroxylation of steroids at unactivated carbon centers, Case Study. -2 hours

4. Bioremediation and Biological Methods for Pollution Control:
Environmental remediation: Bioremediation and biodegradation - molecular biological approaches to sustainable development. -2 hours
Bioremediation of fossil fuels like oil, coal, pesticides and PCBs. -1 hour
Anaerobic and aerobic degradation, site characterization, treatability assessment, remediation technology selection -2 hours
Design of in situ remediation techniques, phytoremediations, Case Study. -2 hours
Environmental enhancement: Positive intervention: molecular biological approaches to increasing biochemical tolerance (crop protection, fertilizers) -2 hours
Clean technologies: biotechnological alternatives to present energy sources -2 hours
and commodity production; -1 hour

References:

PRESCRIBED BOOKS:

1. Doble Mukesh, Anil Kumar and Vilas Gajanan Gaikar, Biotransformations and Bioprocesses, Marcel Dekker, New York, USA, 2004.
2. Doble Mukesh and Anil Kumar Biotreatment of Industrial Effluents, Elsevier, USA, 2005.
3. H. G. Davies, D. R. Kelly, R. H. Green and Stanley M. Roberts, Biotransformations in Preparative Organic Chemistry, Academic Press, New York, 1989.
4. Kurt Faber, Biotransformations in Organic Chemistry, Springer Verlag, Berlin, 2018.
5. Pauline M. Doran, Bioprocess Engineering Principles, Academic Press. 1995, ISBN-13:978-0-12-220856-0

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1. Michael L. Shuler and FikretKargi Bioprocess Engineering, Basic concepts, Second Edition, PTR Prentice Hall. 2001, ISBN 0-13-081908-5.
2. Peter Grunwald, Biocatalysis: Biochemical fundamentals and applications, Imperial college Press,2009, ISBN-13 978-1-86094-771-1; ISBN-10 1-86094-771-9
3. Gideon Grogan, Practical Biotransformations: A beginners' guide, First edition, John Wiley & Sons,2009, ISBN 9781405193672.

PCHM-405 E-II (ii): Organic Chemistry of Natural Products

(Elective) (3 CREDITS – 42 Hours)

Course Objectives:

1. To provide an overview of the field of natural product chemistry.
2. Using selected examples, this course describes the process of isolation and identification of natural products from natural sources.
3. The course covers their chemical synthesis, biological activities, and ecological relevance.
4. Special emphasis is given to secondary metabolites related to terpenes, alkaloids and flavonoids.
5. To learn basic principles of organic chemistry through the study of natural products- structure, stereochemistry and synthesis.

Course Outcomes: Upon completion, the student will be able to

1. Predict the biosynthetic pathways of a secondary metabolite.
2. Outline the total synthesis of any metabolite covered in the syllabus.
3. Know the methods for isolation, purification and characterization of secondary metabolites.
4. Solve organic chemistry problems using chemical and spectral methods.

Syllabus:

1. Methods in Natural Product Chemistry:

Techniques used in isolation	-1 hour
Determination of structures of different types of plant secondary metabolites-	-2 hours

2. Biosynthesis:

Introduction to acetate malonate pathway	-1 hour
Acetate mevalonate pathway	-2 hours
Shikimic acid pathway	-2 hours

3. Terpenes and Steroids:

Structure elucidation of citral	-2 hours
Photochemistry of santonin	-2 hours
Synthesis of longifolene	-2 hours
Total synthesis of steroid hormones	-2 hours
Synthesis of Prostaglandins ($PGF_{2\alpha}$)	-2 hours

4. Alkaloids:

Biosynthesis of opium alkaloids: Stereochemistry and rearrangements of morphine	-2 hours
Determination of structure of strychnine	-2 hours
Stereochemistry and synthesis of quinine –	-2 hours
Photochemistry of Colchicine-	-2 hours

5. Oxygen Heterocyclic Compounds: Structure elucidation of flavonoids with a suitable example

(use of colour reactions, UV, MS, ^{13}C&^{1}H NMR)-	-2 hours
Determination of structure of scandenin by spectral methods	-2 hours.

6. Antibiotics:
Reactions of penicillin -2 hours
Total synthesis of anti-cancer antibiotics such as daunorubicin -3 hours

7. Chemical Ecology:
An introductory study:
Chemistry of insects with particular reference to chemical defence mechanisms, pheromones -2 hours
Plant defence chemicals - Allelo - chemicals and Phytoalexins
(examples and their use in agriculture) -2 hours

8. Problem-Solving Sessions: Critical analysis and interpretation of data from current literature concerning natural products. -3 hours

References:

PRESCRIBED BOOKS:

1. N. R. Krishnaswamy, Chemistry of Natural Products – A Unified Approach, University Press, Hyderabad, 1999.
2. K. C. Nicolaou and E. J. Sorensen, Classics in Total Synthesis, VCH, 2014
3. K. Nakanishi et al (Editors) Natural Products, Vols 1, 2 and 3, Academic press 1974, 1975 and 1983.
4. J. Mann, R. S. Davidson, J. B. Hobbs, D. V. Banthorpe and J. B. Harborne, Natural Products, Addison Wesley Longman Limited, 1994.
5. E.J. Corey and Xue-Min Cheng, The Logic of Chemical Synthesis, John Wiley and Sons, 1995.

REFERENCE BOOKS:

1. Coffey (Editor), Rodd's Chemistry of Carbon Compounds, Vols 2 C, D, and E with supplements and volumes 4E, G and H, Elsevier 1974 to1985.
2. J. Apsimon (Editor),Total synthesis of Natural products, Vols I,V and VI Academic Press, 1973, 1983 and 1984.

PCHM 405 E -II (iii): Advanced Aspects of Polymer Chemistry

(Elective) (3 CREDITS-42 Hours)

Course Objectives:

1. To study various methods employed in the synthesis of polymers and develop an understanding of the chemical kinetics and mechanistic aspects that are involved.
2. To develop an understanding of the stereochemistry of polymers, and their thermal and mechanical properties as outlined in the syllabus.
3. To learn about polymer processing, and the additives used in polymer products.
4. To understand polymer stability and polymer degradation in the environment.
5. To understand the applications of polymers in different technologies.

Course Outcomes: Upon completion, the student will be able to

1. Design polymer synthesis schemes.
2. Appreciate polymer structure-property relationship.
3. Solve numerical and structural problems related to systems studied.
4. Identify polymers for different applications.

Syllabus:

1. Condensation Polymerization:

Molecular weight distribution in linear polymerization polyfunctional step reaction polymerization-1 hour
Newer types of step Polymerization-Dendrimers -1 hour
Phenol-formaldehyde, Melamine- formaldehyde, Urea-formaldehyde -1 hour

2. Addition polymerization:

Determination of absolute rate constants - energetic characteristics -1 hour
Auto acceleration -1 hour
General considerations on Living Radical Polymerization -1 hour
Introduction to ATRP and RAFT -2 hours

3. Surfactants in polymerization:

Different types of surfactants -1 hour

4. Polymerization through ionic species:

Anionic polymerization of the carbon-carbon double bond - Block copolymers. -1 hour
Chain transfer in ionic Polymerization-Living polymers -2 hours

5. Theory of copolymerization:

Statistical derivation of copolymer composition equation-kinetics of co-polymerisation. Applications of co-polymerization. -2 hours

6. Stereoregular Polymerization:

Types of stereoisomerism in polymers - Properties of stereoregular polymers -1 hour
Forces of stereo regulations in alkene polymerization, - kinetics -3 hours

7. Polymer Structure and Physical Properties:
Polymer crystallinity -1 hour
Crystalline melting point - Glass transition temperature -1 hour
Factors affecting T_m and T_g -1 hour
Property requirements and polymer utilization: fibers, flexible and rigid plastics, and elastomers -1 hour

8. Mechanical behaviour of Polymers:
Mechanism of deformations and strengthening of polymers:
Deformation of semi-crystalline polymers: mechanism of elastic deformation and mechanism of plastic deformation. Factors that influence the mechanical properties of semi-crystalline polymers -1 hour
Deformation of elastomers -1 hour

9. Polymer Characterization:
Electron microscopy and diffraction, Mass, NMR, -2 hours

10. Polymer Additives: -2 hours
Plasticizers, Antioxidants, heat stabilizers, UV Stabilizers, Flame retarders, Colorants, Curing agents and lubricants.

11. Basics of Polymer Processing: -2 hours
Extrusion, moulding (compression, transfer, injection, thermoforming, blow moulding, reaction injection moulding), calendaring and coating.

12. Polymer Degradation and the Environment: -2 hours
Degradation and stability, Thermal degradation, Oxidative and UV Stability, Chemical and Hydrolytic stability, Effects of radiation, Mechano Degradation; Recycling, Incineration and Biodegradation

13. Polymers for Advanced Technologies:
Membrane science and technology: Membrane separation -membrane preparation-Mechanisms of transport -3 hours
Biomedical engineering and drug delivery: Controlled drug delivery-Gene Therapy-Antimicrobial Polymers-Tissue engineering- Kidney dialysis and artificial organs -3 hours
Applications in electronics and energy: Electrically conductive polymers-Polymeric Batteries-Organic photovoltaic polymers-Electronic Shielding-Dielectrics-Electronic encapsulation -2 hours
Photonic polymers: Nonlinear optical polymers-Light- emitting diodes -1 hour
Sensor applications -1 hour

References:

PRESCRIBED BOOKS:
1. G. Odian, Principles of Polymerisation, 4th Ed., John Wiley & Sons., New Jersey, 2004.
2. H R Allcock, F.W. Lampe and J. E. Mark, Contemporary Polymer Chemistry, 3rd ed., Pearson Education Inc. New Jersey 2003.
3. W. D. Callister Jr. and D. G. Rethwisch, Materials Science and Engineering – An Introduction, 9th edition, 2014, Wiley NJ.
4. C.E. Carraher Jr., Seymour/Carraher's Polymer Chemistry, 5th ed., Marcel Dekker Inc., New York 2000.

5. Joel R Friend, Polymer Science and Technology, 3rd Edition, Pearson Education, New Jersey, 2014.
6. M. Chanda, Introduction to Polymer Science and Chemistry – A Problem Solving Approach, 2nd Ed., CRC Press, USA 2013.

REFERENCE BOOKS:

1. M. P. Stevens, Polymer Chemistry, 2nd ed., Oxford University Press 1990.
2. L. H. Sperling, Introduction to Physical Polymer Science, 4th ed., John Wiley & sons, New Jersey 1993.

PCHM-406: Practical: Computational Applications in Chemistry – II
2 CREDITS
Course Objectives:
1. To familiarize the students with the procedure and principles of molecular docking. 2. To teach the fundamentals of molecular dynamics (MD) and its practical applications. 3. To expose the students to various numerical methods using Scilab. 4. To impart the nuances of statistical analysis to students.
Course Outcomes: Upon completion, the student will be able to
1. Perform molecular docking simulations. 2. Perform molecular dynamic (MD) simulations and interpret the results. 3. Run GROMACS and compute various properties of macromolecular systems. 4. Know the basics of numerical methods and Scilab programming. 5. Perform various statistical analyses.
Syllabus:

1. **Molecular Docking** -9 hours
Basics of Molecular Docking, Types of Docking, Scoring Functions, Performing docking with Auto dock or Autodock Vina or Pyrx, Pymol, MOE

2. **Molecular Dynamics Simulations** -30 hours
Introduction to Molecular Mechanics
Introduction to force fields
Force field parameterization
Basics of Molecular Dynamics Simulation
Energy minimization and MD Simulations
Trajectory generation and structure analysis
Introduction to Gromacs software
Electrostatic Surface Potential in Biomolecules
Solvation in Biomolecules
Hybrid Calculations: Quantum Mechanics/Molecular Mechanics (QM/MM)

3. **Statistical Analysis Using RSoftware** -27 hours
1. Descriptive Statistics – Variables (Numerical-Ratio Scale, Interval Scale, Categorical-Nominal, Ordinate); Data Structures; Central Measures of Tendency-Mode, Median, Mean
2. Measures of Dispersion – Standard Deviation, Variance; Measures of Distribution – Skewness and Kurtosis
3. Data Visualization –Scatter Plot, Bar Plot, Histogram and Pie Chart; Inferential Statistics
4. Regression – Linear, Nonlinear; Correlation - Pearson Correlation, Spearman Correlation, Kendall's Correlation
5. Paired Samples t-test, One-Sample t-test, Two-Sample t-test
6. Analysis of Variance (ANOVA), Normality test of datasets

4. **Numerical Methods Using Scilab Software** -18 hours
1. Introduction to Numerical Methods
2. Determination of Eigenvalues and Eigenvectors of a Square Matrix.
3. Finding derivatives - Numerical Differentiation
4. Solving Integrals - Numerical Integration.
5. Solving Differential Equations Using Euler Method/Runge-Kutta Method.
6. Performing an Exponential Fit and Analysing Residuals

References:

1. K. I. Ramachandran, G. Deepa, K. Namboori, Computational Chemistry and Molecular Modelling Principles and Applications Springer-Verlag Berlin Heidelberg, ISBN-13 978-3-540-77302-3. 2008.
2. Errol Lewars, Computational Chemistry Introduction to the Theory and Applications of Molecular and Quantum Mechanics 3rd Ed., 2004 Kluwer Academic Publishers New York, Boston, Dordrecht, London, Moscow, ISBN: 1-4020-7285-6. 2018.
3. Frenkel D and Berend S, Understanding Molecular Simulations From Algorithms to Applications, 2nd Ed., Academic Press New York, 2002.
4. David C. Young, Computational Chemistry: A Practical Guide for Applying Techniques to Real-World Problems. John Wiley & Sons, Inc. 2011.
5. W. Koch, M. C. Holthausen, A Chemist's Guide to Density Functional Theory - ISBN 3-527-30372-3, 2001.
6. A.C. Norris, Computational Chemistry, Wiley–Blackwell, ISBN-13:978-0471279495, John Wiley, 1981.
7. C. E. Frogberg, Numerical Analysis, 2nd Ed., Addison-Wesley Educational Publishers Inc., Macmillan, 1970.
8. M.J. Maron, Numerical Analysis - A Practical Approach, 2nd Ed., ISBN-13:978-0534982119,Macmillan Publishing Company, 1991.
9. H. M. Antia, Numerical Methods for Scientists and Engineers, 3rd Ed., ISBN-13:978-3764367152, Tata McGraw Hill, 2002.

PCHM-407: Project work

8 CREDITS

Course Objectives:

1. To train students towards designing research experimental plans with resource optimization and time management.
2. To offer the hands-on experience of performing research experiments.
3. Nurture the key scientific skills of data analysis, documentation and presentation of experimental research data in the form of a brief thesis and slide deck presentation.

Course Outcomes: Upon completion, the student will be able to

1. Design probable experimental plans for an identified research problem based on the availability of resources.
2. Perform research experiments with the knowledge of laboratory and instrument related safety precautions.
3. Analyse the experimental data and results.
4. Document and present the outcomes of the research project in a coherent and scientific manner.

Submission of dissertation and comprehensive viva of the project work:

The final project report is submitted to the university as a dissertation in prescribed format. The department panel consisting of project supervisors, Head of the department and Dean of research conduct a comprehensive viva voce after a slide deck presentation by the student. The assessment for the Project Work includes 1/5th weightage for the review of the preliminary report submitted by the student at the end of the 3rd semester + 1/5th weightage for the Project Work viva-voce conducted at the end of the 4th semester + 3/5th weightage for the double evaluation of the Project Report (by one internal and an external examiner) submitted at the end of the fourth semester.