SRI SATHYA SAI INSTITUTE OF HIGHER LEARNING

(Deemed to be University)

Syllabus for
M.Sc. in Chemistry

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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 papers (including Mathematics for Chemistry) spread over four 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 a rigorous training in all the major branches of chemistry. In the final semester, advanced emerging fields of research are being introduced in order to enable the students to have a good knowledge of current trends in research across the domains of chemistry. Electives in frontier and inter disciplinary areas are being offered in the third and fourth semesters. 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. Some inter departmental electives are also introduced in the course. 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

- Teach basic concepts and educate to retain knowledge
- Synergy between theoretical and experimental knowledge
- Training in relevant computational and experimental methods

Inspiring design and innovation

- Establish a learning program that aids an inventive culture
- Design and model molecules that mimic bio-relevant molecules in biological processes
- Educate about how chemistry is the essence of all living systems and physical processes

Create and Collaborate

- Create materials for energy storage, drug delivery, molecular imaging and water purification
- Remove barriers between conventional branches of Chemistry and explore collaboration within and outside of SSSIHL
- Mould students into research-oriented scientists with noble ambitions.

Values

- Inspire research with relevance and applications to society
- 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 Outcome

The Bachelors and Masters programmes offered by the department of chemistry equips students with in-depth understanding of the fundamentals in all the major domains of Chemistry. It aims to deliver to the graduate a right mix of theory, application, instrumentation, computation and experimentation, in Chemistry, in tune with the latest advancements in the field. The skills, knowledge and kindled spirit of research is designed to inspire the student to explore the vast world of chemistry.

Program Specific Outcome

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, bio-remediation, 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.

Course Outcomes

Under-graduation

Starts with the key principles of atomic and molecular theory and leading to the analytical principles of Thermodynamics, Kinetics and Equilibria. Introduces spectroscopy and consequent applications in Surface Chemistry, Synthetic Organic Chemistry and Inorganic chemistry, culminating in the chemistry of Biological Molecules. Finally, the advanced electives provide exposure to the evolving aspects of Quantum Chemistry, Environmental and Green Chemistry, Theoretical Aspects of Spectroscopy, and Materials of Industrial Importance, and reveal the wide realm of Chemistry to the young graduate and gives the thirst to explore more.

Post-graduation

Provides advanced courses in Quantum Chemistry and Group Theory, Analytical Chemistry, Chemical Kinetics and Surface Chemistry, Polymer Chemistry & Special Topics from Physical Chemistry and Synthetic Organic Chemistry. In addition to these, the courses in Computational Applications in Chemistry – at beginner and advanced levels – coupled with the 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 job in industry**.**

Attainment of POs, PSOs, and COs

We keep a tab on the alumni placement and their performances across the world to informally evaluate the success of our program outcomes. The internal assessment instituted by the department to conduct the viva-voce along with the continuous internal assessment instituted by the University along with the semester exams grade the performance of the students for the program specific outcomes and the course outcomes. A timely continuous look at the overall performance of the student leads to appropriate measures.

DEPARTMENT OF CHEMISTRY

SCHEME OF INSTRUCTION AND EVALUATION

M.Sc. (CHEMISTRY)

(Effective 2020/21 batch onwards)

Paper Code	Title of the Paper	Credits	Hours	Modes of Evaluation	Types of Papers	Maximum Marks
Semester I						
PCHM-101(i)	Quantum Chemistry and Group Theory	**4**	4	IE2	T	100
PCHM-101(ii)	Mathematics for Chemistry	**Non-Credit**	1	I	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	Practicals: Coordination Chemistry (Preparation and Analysis)	**2**	6	I	P	50
PCHM-106	Practicals: Analytical Chemistry	**2**	6	I	P	50
PCHM-107	Practicals: 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
		20 credits	**34** Hours			**600** 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	Practicals: Inorganic Chemistry	**2**	6	I	P	50
PCHM-206	Practicals: Physical Chemistry	**2**	6	I	P	50
PCHM-207	Practicals: 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	**3**	3	IE2	T	100
PCHM-303	Elective-I	**3**	3	IE2*	T	100
PCHM-304	Elective–II (Inter-Departmental Electives)	**3**	3	IE2*	T	100
PCHM-305	Practicals: Computational Applications in Chemistry-I	**2**	6	I	P	50
PCHM-306	Project work (Interim Review) **	**Non-Credit**	12	-	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–III (Inter-Departmental Electives)	**3**	3	IE2*	T	100
PCHM-405	Elective–IV (Inter-Departmental Electives)	**3**	3	IE2*	T	100
PCHM-406	Practicals: 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	**77** credits	**130** Hours			**2400** marks

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 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.

The elective papers are listed below:

Elective Papers offered in the Third and Fourth Semesters

THIRD SEMESTER (Choose any ONE paper from each of the following electives):

ELECTIVE -I.

PCHM-303 E-I (i) Synthetic Organic Chemistry
PCHM-303 E-I (ii) Nanoscience and Nanotechnology

ELECTIVE – II: (Interdepartmental elective)

PCHM-304 E-II (i) Theory and Application of Physical Methods in Chemistry
PCHM-304 E-II (ii) Materials and their Characterization
PPHY- EL 12 Biomaterials

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

ELECTIVE – III: (Interdepartmental elective)

PCHM-404 E-III (i)	Environmental Chemistry
PCHM-404 E-III (ii)	Advanced aspects of applications of group theory in Chemistry
PBIO-404 E-IV (BT-4)	Environmental Biotechnology

ELECTIVE – IV: (Interdepartmental elective)

PCHM-405 E-IV (i)	Biocatalysis for Industry and Environment
PCHM-405 E-IV (ii)	Organic chemistry of natural products
PPHY-EL 21	Graphene and 2-dimensional materials

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

PCHM-101(i): Quantum Chemistry and Group Theory

(4 CREDITS – 56 Hours)

Course Objectives:

1. To teach the fundamentals of quantum chemistry like concept of operators, eigenvalues, eigen functions etc.
2. Setting up and solving 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 eigenvalues, eigenfunctions etc.
2. Set up Schrodinger equation and solve it for simple systems.
3. Determine the various symmetry operations for diverse molecules, using 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, Wein's Displacement Law, Planck's Distribution Law, Dulong and Petit Law -1 hour

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

Hermitian Operators, Commutative Operators -1 hour

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 -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
Hydrogen like Orbitals, Born-Oppenheimer Approximation -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 -2 hours
Perturbation Method – Introduction, First Order Perturbation Theory -1 hour
Second Order Perturbation Theory -2 hours

7. Many Electron Atoms

Atomic Hours; Hartree-Fock and Configuration Interaction Wave Functions for Helium Atom -1 hour
Solution by Self-Consistent Field Method, Anti-Symmetrization of Wave Functions -1 hour
Slater Determinants, Hartree-Fock Roothan Method -1 hour
Spin Statistics Theorem, Correlation Energy, Condon Slater Rules -1 hour

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 -1 hour
Introduction to SCF, SCF Calculation on H_2, Basis Sets – Polarization Terms -1 hour
Comparison of MO and VB theories -1 hour
Virial Theorem -1 hour
Huckel Π electron theory and its application to ethylene, butadiene and benzene -1 hour

9. Theoretical Calculations

Semi Empirical Methods – Parameterization, Approximations; -1 hour
Molecular Mechanics Methods – Force Fields; -1 hour
Ab Initio Calculations -1 hour
Electron Correlation Methods - Correlation Energy, Configuration Interaction -1 hour
Moller-Plesset (MP) Perturbation Theory -1 hour
Coupled Cluster Methods -1 hour
Density Functional Theory -1 hour
Relativistic Effects -1 hour

10. 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. -1 hour
Application to Molecular Orbitals (O_h, T_d, D_{4h}), hybrid orbitals (σ and л), determination of Hybridization of molecules -2 hours

Deductions of normal modes of vibrations for polyatomic molecules (non-linear) - Cartesian coordinates method, internal co-ordinates method-general method -2 hours Applications to IR and Raman spectra, Selection rules for electronic, IR and Raman spectra, Application to interpretation of electron density maps in X-ray Crystallography -2 hours
References:

PRESCRIBED BOOKS:

1. Donald A. McQuarrie, Quantum Chemistry, Second edition, University Science Books, California, 2008.
2. Levine, Quantum Chemistry, 7^{th} Ed, Prentice Hall 2013.
3. F. L. Pilar, Elementary Quantum Chemistry, Dover Publications, 2nd Ed., Inc. NY, 2003.
4. A. K. Chandra, Introduction to Quantum Chemistry, 4^{th} Ed., Tata McGraw Hill, 1994.
5. F. A. Cotton, Chemical Applications of Group Theory, 3^{rd} Ed., Wiley 1994.
6. K.V. Raman, Group theory and its applications to chemistry, McGraw Hill Education, 1990
7. P.W. Atkins, T.L. Overton, J.P. Rourke, M.T. Weller, and F.A. Armstrong, Shriver & Atkins' Inorganic chemistry, Fifth edition, W.H. Freeman and company, 2010

REFERENCE BOOKS:

1. P. W. Atkins and R. S. Friedman, Molecular Quantum Mechanics, 5th Ed., Oxford Univ. Press, 2010.
2. M. W. Hanne, Quantum Mechanics in Chemistry, 3^{rd} Ed. Benjamin 1981.
3. S. F. A. Kettle, Symmetry and Structure, 3^{rd} Ed., Wiley 2007.
4. Lucjan Piela, Ideas of Quantum Chemistry, 3^{rd} Ed., Elsevier, Amsterdam, 2020.
5. R. K. Prasad, Quantum Chemistry, 3^{rd} Ed., Wiley Eastern, 2006.

PCHM-101(ii): Mathematics for Chemistry

(Non-Credit Course)

Course Objectives:

1. To apply critical intuition in the solving of applied phenomena, using the mathematical knowledge of calculus to formulate problems of science.
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 gain comfort with the use of various mathematical skills for future applications.

Course Outcomes: At the end of the course, the learners should be

1. confident to use mathematical tools of linear algebra and ODEs in various disciplines of chemistry.
2. at ease in using matrix algebra in linear equations, to solve problems using analytical methods.
3. able to rationalize mathematical, statistical and probability distributions for any given challenge.

Syllabus:

1. Introduction to numbers (real numbers, complex numbers) 1 h
2. Functions: properties of functions-operations on functions-Dirac delta function 2 h
3. Calculus: Basics of differentiation-Basics of integration-Differential equations 2 h
4. Determinants and Matrices: Matrix operations-properties of matrices 3 h
5. Operators: linear operators-Hermitian operators 1 h
6. Review of vector space: Introduction to vectors-vector operations-vector space-basis vectors-linear transformations-orthogonality properties 2 h
7. Matrix Eigen value problems and Eigen functions 1 h
8. Probability and statistics 1 h
9. Series and limits 1 h

There should not be any external examination on this mathematics course.

References:

1. D.A. Mcquarrie, Quantum Chemistry, Oxford University Press, Second edition, 2007.
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)
4. Erich Steiner, The Chemistry Maths Book, Oxford University Press (2008)
5. Paul Monk, Maths for Chemistry: A Chemist's Toolkit of Calculations, Oxford University Press (2006)
6. Robert G Mortimer, Mathematics for Physical Chemistry, 3edn. Academic Press (2005)
7. 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 statistical treatment of data, chromatographic separations and solvent extractions
3. To study various advanced separation techniques crucial for both qualitative and quantitative analysis of samples
4. To extend existing analytical methods to new types of samples, and to learn about their applications in the areas of radio analytical chemistry and photoelectron chemistry.
5. To study the instrument layout and components of some instrumental techniques

Course Outcomes: Upon completion the student will be able to

1. Understand the theoretical principles behind the techniques covered in the course
2. Learn important analysis methods to analyse and separate samples at macro and microscale
3. Realize the applicability, advantages, and disadvantages of each method studied
4. Understand the layout and working of each instrument

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
Instruments Architecture and methods of detection, Eminin software - Demo -3 hours

2. Separation Techniques:

Super critical fluid chromatography- Principle and instrumentation-Applications of SCF -2 hours
Super critical 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 electrode, solid electrodes,
Chemically modified electrodes and microelectrodes- -1 hour.
Voltammetry - pulse voltammetry (normal, differential, square wave, stair case 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 hour
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 - Electro chemical monitoring of photolytic intermediates - Electrochemiluminescence-	-2 hours

6. Instrumentation:

UV - Visible, IR, luminescence,	-2 hours
NMR, Mass spectrometer	-2 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. D. A. Skoog, D. M. West and F. J. Holler, Fundamentals of Analytical Chemistry, Saunders College Publication, New York - 9th Ed., 2013.
3. G. D. Christian, Analytical Chemistry, 7th Ed. John - Wiley & Sons 2013.
4. P. T. Kissinger and W. R. Heineman, Laboratory Techniques in Electro Analytical Chemistry, 2nd Ed., Marcel Dekker Inc. New York 2016.
5. J. Tolgyessy and M. Krys, Radio Analytical Chemistry Vol I & II, Ellis Horwood Ltd, 1989
6. Joseph Wang, Analytical Electrochemistry, 3rd Ed., Wiley VCH, 2006.

REFERENCE BOOKS:

1. R. M. Smith, Supercritical Fluid Chromatography, The Royal Society of Chemistry 1988.
2. D. L. Andrews, Perspectives in Modern Chemical Spectroscopy, Springer Verlag, 1990
3. R. A. Day Jr., A.L. Underwood, Qualitative analysis, 6th Ed., Prentice Hall of India, 1991.
4. Vogel's Text book of Quantitative Inorganic Analysis (revised copy), 5th Ed., ELBS, 1994.

PCHM-103: Coordination Chemistry

(3 CREDITS - 42 Hours)

Course Objectives:

1. To understand the key theories of coordination compounds including the energy level diagrams of various systems
2. To be able to use the theories of metal-ligand bonding to understand the spectral and magnetic properties of coordination compounds.
3. To understand the kinetics and mechanisms of reactions involving octahedral and square planar metal complexes.
4. 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 while in the presence of crystal field, and understand their energies and field strengths. (Octahedral, tetrahedral, and square planar).
2. understand the origin of colours in various coordination compounds
3. calculate ligand-field stabilization energies.
4. understand the mechanisms of thermal systems by knowing the electronic nature of the excited states.

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 – -1 hour

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 - Irwing-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 anti-ferromagnetism) - 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

Relaxation processes of excited states - emission from excited states: $[Cr(en)_3]^{3+}$ ion, $[Ru(bpy)_3]^{2+}$ ion excited state electron transfer processes – -1 hour

Brief account on 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, 2nd Ed., (volumes: 1-7), CBS Publishers and Distributors Pvt. Ltd. **2010.**
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. F. Basolo and R.G. Pearson, Mechanisms of Inorganic Reactions, 2nd Ed., Wiley Eastern, 1977.
5. F. Basolo and R. Johnson, Coordination Chemistry, W. A. Benzamin Inc., 1964.
6. D. Banerjea, Coordination Chemistry, 3rd Ed., Tata-McGraw-Hill 2009.

7. David Nicholls, Complexes and First Row Transition Elements, Macmillan 2017.
8. O. Kahn, Molecular Magnetism, Wiley VCH, 1993.

Reference Books:

1. V. Balzani & V. Carasitti, 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. Martin L. Tobe and John Burgess, Inorganic Reaction Mechanisms, Longman, 1999.
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 about aromaticity, non-aromaticity and anti-aromaticity using Molecular Orbital Theory.
2. To elucidate the reactivity and aromaticity in heterocyclic compounds.
3. To have an in depth understanding about the conformational studies in cycloalkanes supplemented by NMR. This also includes stability studies of transannular 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 about the aromaticity of organic system/moiety.
2. Solve numerical problems related to systems studied.
3. Predict and identify the stability and optical activity of any organic system having got a strong background in conformation and configuration stereochemistry.

Syllabus

1. Resonance and Aromaticity

The concept of resonance as distinct from the phenomenon of tautomerism - a review with appropriate examples. -1 hour

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

Structure and chemistry of Dendralenes and Radialenes. -1 hour

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

An introduction to computer assisted energy calculations of aromatic, anti-aromatic and non-aromatic systems using ab initio molecular orbital packages/programs (PC Spartan & Hyperchem lite) - 2 hours.

Further illustrations of Huckel's rule - The simplest aromatic system - The cyclopropenyl carbocation. -1 hour

Cyclobutadiene and cyclooctatetraene - Molecular orbital pictures to demonstrate their anti-aromaticity - Jahn Teller effect. -1 hour

Non-benzenoid aromatic hydrocarbons derived from cyclo pentadienyl carbanion - The Fulvenes and Fulvalenes. -1 hour

Cycloheptatrienyl carbocation - tropone and tropolones. -1 hour

Annulenes - aromatic and anti - aromatic systems - ring current and its effect on proton magnetic resonance spectra. -1 hour

Bicyclic and polycyclic aromatic systems - Azulenes. -1 hour

Dewar's perturbation of molecular orbitals approach to the prediction of aromaticity, non-aromaticity and anti-aromaticity of conjugated cyclic systems. Alternate and non-alternate hydrocarbons and the concept of union. -2 hours

Heteroaromatic compounds - comparative aromaticity of five membered and six membered heterocyclic compounds containing one heteroatom. - An introduction with sydnones as example. -2 hours

2. Valence bond tautomerism and rigid structures:

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

The chemistry of fullerenes with particular reference to buck minister fullerene - C60 Determination of structure, reactions and applications. -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

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 PMR 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 spirans. -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 diastereo isomers - 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 -1 hour

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

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

References

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1. L. N. Ferguson, The Modern Structural Theory of Organic Chemistry, Prentice Hall 1966.
2. R. A. Y. Jones, Physical and Mechanistic Organic Chemistry, 2nd Ed., Cambridge University Press, 1984.
3. William J. Le Noble, Highlights of Organic Chemistry, Marcel Dekker Inc. New York, 1974.

4. Michael B. Smith & J. March, Advanced organic chemistry, 6th Ed., John Wiley & Sons, Inc, NewYark,2006.
5. E. L. Eliel, Stereochemistry of carbon compounds, Tata Mc Graw Hill, 1962.
6. D. Nasipuri, Stereochemistry of organic compounds principles and applications, Wiley Eastern, 1991.
7. J. Clayden, N. Greeves, S. Warren, P. Wothers, Organic chemistry, Oxford University Press, 2005.(Pg no 468-470,858-861).

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1. S. H. Pine, J. B. Hendrickson, C. J. Cram and G. S. Hammond, Chapters 6 and 13 in "Organic Chemistry", 4th Ed., Mc Graw Hill, Kogakusha ,1980.
2. Streitweiser Jr., Molecular Orbital Theory for Organic Chemists, John Wiley & Sons, 1961.
3. W. J. Hehre, A. J. Shusterman, W. W. Huang, A Laboratory Book of Computational Organic Chemistry, Wavefunction Publications, 1996.
4. L. N. Ferguson, The Modern structural theory of organic chemistry, Prentice Hall of India, 1966.
5. J. Dale, Stereochemistry and conformational analysis, Verlag Chemie, 1978
6. E. B. Ramsay, Heyden, Stereochemistry, 1981.
7. J. A. Marshall, Carbon-Carbon and Carbon - Proton NMR couplings - Applications to Organic Stereo-chemistry and Conformational analysis, Florida Verlag Chemie, 1983.
8. K. Mislow, Stereochemistry, Benzamin Kummins publications, 1965.
9. J. Reney and J. A. Robinson, Stereospecificity in organic chemistry and enzymology, Florida, Verlag Chemie-Monographs in Modern Chemistry, 1982
10. Fullerenes, Ed George S Mammond, Valerie J Cook, ACS Symposium series, 4 :1, 1982.

PCHM-105: Practicals: Coordination Chemistry (Preparation and Analysis)

2 CREDITS

Course Objectives:

1. To prepare inorganic 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 knowhow 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:** 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 lron-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-Ethylene diamine complex: Slope-ratio method
9. **Photochemistry Experiment:** Potassium Trioxaltoferrate 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

References:

1. A. I. Vogel, A Text book 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: Practicals: 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 milli-molar to micro molar concentrations.
3. To introduce different electro-analytical techniques of varied industrial and academic importance

Course Outcomes: At the end of the course, the learners should be able

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

Syllabus:

1. Manganese determination by titrating with permanganate in neutral pyrophosphate solution.
2. Estimate concentration of H_2SO_4, CH_3COOH and $CuSO_4$ by conductometric titration with NaOH.
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. Titration of pure solutions of KI, KCl and KBr and their mixtures against AgNO3.
6. One step synthesis of metal nanoparticles using water soluble polymers and their applications
7. Separation of mixture of compounds using HPLC
8. Separation of mixture of compounds using GC
9. Quantification of Caffeine/Polyphenols in various teas using HPLC
10. Synthesis of metal-polyphenolic complexes for detection of anions
11. Estimation of metal content in a sample using AAS

References:

1. Donald T. Sawyer, William R. Heineman & Jalice M. Beebe, Chemistry experiments for Instrumental Methods, John Wiley & Sons, 1984.
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: Practicals – Organic Qualitative Analysis
(Mixture Separation & 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 practice derivative preparation as a method to confirm presence of functional groups.
3. To practice column chromatography for the separation of binary and ternary mixtures of organic compounds
4. To use Thin-Layer Chromatography for analysis of simple APIs available in market

Course Outcomes: Upon completion the student will be able to

1. separate binary organic mixtures and identify functional groups in the components
2. apply techniques learnt to organic compound mixtures obtained during synthesis protocols

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. Column Chromatography based separation

Separation of binary and ternary mixtures of organic compounds using column chromatography.

3. TLC Analysis

TLC analysis of some patent medicines.

4. Paper Chromatographyl– Separation of chlorophyll or dyes

References:

1. A.I Vogel, Elementary Practical Organic Chemistry Part II, Qualitative Organic analysis, 2nd Ed, CBS publications, 1987.
2. V K Ahluwalia and S Dhingra, Comprehensive Practical Organic Chemistry – Qualitative Analysis, University Press, India 2000.
3. C. M. Garner, Techniques and Experiments for Advanced Organic Laboratory, John Wiley and Sons, 1997
4. Eigen Stahl, Thin Layer chromatography - Laboratory Work book 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. know the role of different trace metals present in biological systems
3. know the structure and function of important metalloenzymes
4. understand the mechanism of action of metalloenzymes in various biologically important functions

Syllabus:

Structural Inorganic Chemistry:

Synthesis, Reactions, Structure and Bonding in:

Catenated compounds: Catenation - Heterocatenation, Intercatenation -2 hours

Isopolyanions and Heteropoly anions. -2 hours

Ring compounds: Borazines - Phosphazines, Polyphosphazines-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

Inorganic polymers: Synthesis, structure and applications of the polymers

Polyphosphazenes, -1 hour

Polysilanes -1 hour

Polysiloxanes -1 hour

Metal chelate polymers. -1 hour

Inorganic polymers that contain phosphorous, Boron and Sulphur -1 hour

Bio-Inorganic chemistry:

New perspectives and biological roles of essential trace elements. -1 hour

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

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

Metalloproteins - Metalloenzymes: The characterization of metal - binding sites -1 hour
Carbonic anhydrase – Carboxy peptidase – -2 hours
Super oxide 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

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

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

Metal Ion Folding and Cross-linking of Biomolecules:
Metal-ion stabilisation of protein structure and nucleic acid structure -1 hour
Protein binding to metallated DNA -2 hours
Metal-organised structures as probes for conformation -1 hour

References:

PRESCRIBED BOOKS:

1. J. E. Huheey, E. A. Keiter and R. L. Keiter, Inorganic Chemistry, Harper Collins, 4th Ed., 1993.
2. F.A. Cotton and G. Wilkinson, Advanced Inorganic chemistry, 5th Ed., John Wiley, 5th Ed., New York, 1988.
3. A.F Wells, Structural Inorganic chemistry, 5th Ed., Oxford science publications, 1987.
4. N.N. Greenwood and A. Earnshaw, Chemistry of the elements, 2nd Ed., Buttorworth- Heinemann, 1997.
5. J.E. Mark, H.R. Allcock and R. West, Inorganic Polymers, Prentice Hall1992.
6. M.N. Hughes, Inorganic Reactions of biological processes, John-Wiley, 2nd Ed., New York 1981.
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8. J. A. Cowan, Inorganic Biochemistry - An Introduction, VCH, 1993.
9. 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.

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, as specified in the syllabus.
3. Study of reaction mechanisms using chemical kinetics
4. To study kinetics of catalytic reactions, photochemical reactions, radiation chemical reactions and fast reactions.
5. To develop an understanding of the chemistry of surfaces, physisorption and 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 learnt, 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
Extensions of transition state theory - microscopic reversibility.	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 - Ion-dipole and Dipole - Dipole reactions	1 hour
Extra thermodynamic relationships - Isokinetic relationship	1 hour

4. Composite Reactions:

Types of composite mechanisms - rate equations for composite mechanisms	1 hour
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 combination -Hydrogen - oxygen reaction.	1 hour

5. Photochemical and Radiation Chemical Reactions:

Photochemical reaction - Laser photochemistry - Photosensitisation - Radiation Chemical reactions 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
Transient - Phase kinetics, Sigmoid kinetics - kinetics of bacterial growth 1 hour

7. Isotope Effects:

Equilibrium, Primary and Secondary Kinetic Isotope effects 1 hour

8. Fast Reactions:

Relaxation kinetics - Basic principles of chemical relaxation methods 1 hour
Chemical relaxation in two step and multi-step reactions 1 hour
Experimental methods for the study of relaxation kinetics and applications: Temperature jump method 2 hours
Diffusion controlled reactions, Fluorescence quenching, Common ion inhibition 2 hours
Flash photolysis and introduction to Time resolved Pico/femto second methods 2 hours
(e.g. introduction to Time Correlated Single Photon Counting and FRET)

<u>SURFACE CHEMISTRY:</u>

9. Adsorption of gases and vapors 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

10. Langmuir Blodgett Films:

Structure and characterization mixed LB film, studies of the LB deposition process 1 hour

11. Chemisorption and Catalysis:

Thermodynamics of adsorption, Chemisorption - the molecular view - Chemisorption isotherms 1 hour
kinetics of Chemisorption - The Chemisorption bond. 1 hour

12. 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. K.J. Laidler, Chemical Kinetics, 3rd edition, Pearson Education Inc., 1987.
2. S. K. Upadhyay, Chemical Kinetics and reaction dynamics, Springer USA and Anamaya Publishers, New Delhi, 2006

3. K.A. Connors, Chemical Kinetics - The study of reaction rates in solution, – VCH Publishers, New York 1990.
4. C. Kalidas, Chemical Kinetic Methods, New Age International Publishers, New Delhi, 1996.
5. G.D. Billing and K.V. Mikkalsen, Introduction to molecular dynamics and chemical kinetics. John Wiley & Sons 1996.
6. K.J.Laidler, Physical chemistry with Biological Application, Benjamin Cummings Publications Company Inc., Menlo Park, California 1978.
7. A.W. Adamson and A.P. Gast, Physical Chemistry of Surfaces, 6th Ed. John Wiley & Sons New York 1997.
8. J, O, M Bockris, A. K. N. Reddy, M. Gamboa-Aldeco, Modern electrochemistry, Volume 2A – Fundamentals of Electronics, 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. 1986.

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 partition function and its use in 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, concept of ensemble and types, ensemble average, ergodicity, configuration, thermodynamic probability etc
2. Familiar with the concept of 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 and Implications -1 hour

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

3. Classical Ensembles

Configurations and Weights; Statistical Ensembles: Concept of an Ensemble, Ergodicity, Microcanonical Ensemble; Canonical Ensemble: Boltzmann Distribution, Equipartition Theorem, Internal Energy and Heat Capacity of the Canonical Ensemble; Grand Canonical Ensemble -2 hours

4. Entropy

Swendsen's Postulates of Thermodynamics

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

Concept of Irreversibility, Entropy and Information – Gibbs Entropy, Von Neumann Entropy, Shannon Entropy -1 hour

5. Quantum Ensembles

Quantum Canonical Ensemble - Quantum Partition Function -1 hour

Quantum and Classical Statistics -, Bose-Einstein Statistics, Fermi-Dirac Statistics, Maxwell-Boltzmann Statistics -1 hour

Simple Quantum Systems- Spin S = 1=2, Harmonic Oscillator, Einstein and Debye Models of a Crystal -1 hour

6. Partition Function of Gases

Partition Function - Thermodynamic Functions In Terms of the Partition Function -1 hour

Molecular Interpretation of the Basic Laws of Thermodynamics -1 hour

Separation of Contributions

Evaluation of the Partition Function - Translational Partition Function -1 hour
Rotational Partition Function -1 hour
Vibrational Partition Function -1 hour
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

7. Entropic Elasticity - Ideal Chain Model, Random Walk, Conformational Entropy and Free Energy-2 hours

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

9. Electrodics:
The Concept of Over Potential, 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 – Transient Behavior of Interfaces -2 hours
Determining the Step Wise Mechanism of an Electrodic Reaction, Current Potential Laws for Electro Chemical Systems. -2 hours

10. Applications:
Electrodic Reactions of Special Interest – Electrocatalysis – Influence of Various Parameters. -1 hour
Photo Electrochemistry: 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 -1 hour
Photoelectrocatalysis-The Photoelectrochemical Splitting of Water-The Photoelectrochemical Reduction of CO_2. -1 hour
Electrochemical Energy Conversion – Electricity Storage. -1 hour
Enzymes as Electrodes. -1 hour
Electrochemical Sensors-Electrochemical Biosensors-Gas Sensors-Solid State Devices and Sensor Arrays.
Electrochemical Impedance Spectroscopy -2 hours

References:

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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. Biman Bagchi, Statistical Mechanics for Chemists and Materials Science, CRC Press, Taylor and Francis Group, 2019.
4. J. O. M. Bockris and A. K. N. Reddy, Modern Electrochemistry, Volumes 1 & 2, Plenum Press, New York. 1988.
5. J. O. M. Bockris and A. K. N. Reddy, Modern Electrochemistry 2B, 2nd Ed., Kluwer Academic/Plenum Publishers, New York, 2000.
6. Allen J. Bard, Larry R. Faulkner, Henry S. White, Electrochemical methods –Fundamentals and Applications, John Wiley & Sons, Limited, 2020

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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. J. Goodisman, Electrochemistry Theoretical Foundation, John Wiley Sons, 1987.
6. Christopher M. A. Brett, Ana Maria, Oliveira Brett, Electrochemistry: Principles. Methods and Applications, Oxford University Press, Oxford, 1993.
7. Philip H. Reiger, Electrochemistry, Prentice-Hall International, Inc., 1987.
8. 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 appropriate reaction mechanism.

Syllabus:

1. Nucleophilic addition to the carbonyl group:

Hydride transfer reactions, stereochemistry of hydride reduction -1 hour
Clemmenson & Wolff Kishner reductions -1 hour
Crossed and intramolecular Cannizaro 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- -1hour
Acyloin condensation and its usefulness in the synthesis of large ring compounds -1hour
Mannich reaction and Ritter reaction -1hour

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 - Hack 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 syntheses & 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)- -2 hours,
Stevens, Somelet and Wittig rearrangements- -1 hour
The benzidene 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-1hour;
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. Carey and Sundberg, Advanced organic chemistry, 5th. Ed., Part B, Plenum Press, 2012.
2. J. Clayden, N. Greeves, S. Warren, P. Wothers, Organic chemistry, Oxford University Press, Sec. Ed. 2005.
3. J. March, Advanced organic chemistry, 6th Ed. Wiley - Interscience, 2006.
4. R.A.Y. Jones, Physical and Mechanistic Organic Chemistry, 2nd Ed., Cambridge University Press, 1984.
5. Herbert O. House, Modern Synthetic Reactions, Benjamin/Cummings, 2nd. Ed. 1972.
6. S. N. Mukherji, Pericyclic reactions, Macmillan, 1979.
7. P.S. Kalsi, Organic reactions and mechanisms, 3rd Ed., New Age International Publishers 2010.

Reference Books:

1. William D. Dauben et al., Organic reactions, Eds. Vol.1 to 6 and 28 - 31 John Wiley &Sons, 1947 -1984.
2. R.O.E Norman, Principles of organic syntheses: 2nd Ed., part B, Methusan, 1978.
3. H. Maskill, The physical basis of organic chemistry: Oxford science publications, 1985.

PCHM-205: Practicals: 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. Techniques for water quality monitoring

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 acac and its applications in analysis

Nano-Science

8. Frugal science - Synthesis and characterization of Carbon Dots from kitchen waste
9. Floral synthesis of silver nanoparticles

Water Analysis

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

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 Ed G. Svehla Orient Longman 1982.
3. N.K. Udaya Prakash et al. Asian Journal of Chemistry; Vol. 27, No. 11 (2015), 4089-4091
4. R. Sai Sathish et al. Spectrochimica Acta Part A 66 (2007) 457–461
5. A.L.Himaja et al. J Fluoresc (2014) 24:1767–1773
6. https://ocw.mit.edu/courses/chemistry/5-310-laboratory-chemistry-fall-2017/labs/MIT5_310F17_Ferrocene_Lab.pdf
7. Christina Larson et al. A Comparison of Two Syntheses of Tetraphenylporphyrin. 2013
8. https://core.ac.uk/download/pdf/83550382.pdf
9. Kuen-Song Lin et al. International Journal of Hydrogen Energy 37(18):13865–13871, 2012
10. Paul O'Brien J. Chem. Educ. 1982, 59, 12, 1052
11. M. S. Shalaby et al. Frontiers of Chemical Science and Engineering 7(3):329-337, 2013

PCHM-206: Practicals: Physical Chemistry
2 CREDITS

Course Objectives:

1. To learn physical chemistry principles using experiments
2. To learn to prepare nanoparticles and study its 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 work station

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 kinetics of their growth
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 in a position to operate a fluorimeter
5. explain the electrochemistry chemistry principles behind the experiments and design such experiments and interpret the findings

Syllabus:

1. **Excited state acidity constant measurement:** Determination of excited-state acidity constant of 2-Napthol 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 using Langmuir adsorption isotherm

References:

1. Neidig and Strattom, Modern Experiments for Introductory Chemistry, 2nd Ed., Reprinted from

Journal of Chemical Education, 1989.
2. G. Peter Matthews, Experimental Physical Chemistry, Clarendon Press, 1987.
3. A. M. Halpern, Experimental Physical Chemistry, 3rd Ed., W. H. Freeman, 2006.

PCHM-207: Practicals: Organic Synthesis (multistep) and Spectral Analysis

2 CREDITS

Course Objectives:

To give hands-on experience in carrying out various types of organic reactions including addition, elimination, condensation and functional group protection reactions.

Course Outcomes: Upon completion the student will be able to

Gain the skills and expertise to design and carry out organic reactions performed during the course and use it 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 annelation, 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:

1) Reactions of Indole: The Mannich and Vilsmeier-Haack reactions
2) Enamine reaction: Chiral organic catalysis using proline.
3) Preparation of E-diphenylethene (stilbene) with ylide generation under phase transfer conditions (Benzylchloride ------> Phosphonium salt ------> Stilbene)
4) Cyclohexanol to cyclohexene ------> 2-Br Cyclohexanol to cyclohexene epoxide ------> trans-cyclohexane 1,2-diol
5) Ethyl acetoacetate ------> Ethylene glycol ketal ------> Reduction of COOEt group
6) Achiral and Chiral Reduction of ethyl acetoacetate.
7) Synthesis of β-hydroxy carbonyl compounds by Asymmetric Organo catalysis
8) 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., Vogels 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 mechanisms of various preparative methods and reactivity of various 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 - Cyclometallation reaction -2 hours

8. Physical Methods in Organometallic Chemistry -2 hours

NMR spectroscopy, IR spectroscopy and Crystallography

9. Catalysis by Organometallic Compounds:

Homogenous catalysts: Hydrogenation - Wilkinson’s catalyst, Tolman’s catalytic loops -1 hour
Hydroformylation (oxo process), Cativa process, Buchward-Hartwig Reaction -1 hour
Synthesis gas, water gas shift reaction -1 hour
Olefin metathesis (Grubb’s and Shrock’s catalyst) -1 hour
Heterogenous catalysts: Fischer-Tropsch process and Mobil process -1 hour
Ziegler-Natta polymerization, oligomerization -1 hour

References:

PRESCRIBED BOOKS:

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.
4. R. C. Mehrotra and A. Singh, Organometallic Chemistry, 2nd Ed., Wiley Eastern Ltd, 2004.
5. E. Huheey, E. A. Keiter and R. L. Keiter, Inorganic Chemistry, 4th Ed., Harper Collins 2006.
6. F. A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, 6th Ed., Wiley 1999.
7. N. N. Greenwood and A. Earnshaw, Chemistry of the Elements, 2nd Ed., Butterworth, 1997.
8. I. Haiduc and J. J. Zuckerman, Basic Organometallic Chemistry, WDeG Publishers, 2011.
9. B. Douglas, D. McDaniel and J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Ed; Wiley and Sons, New York, 1994.

REFERENCE BOOKS:

1. K. F. Purcell and J.C. Kotz, Inorganic Chemistry, 2nd Ed., W.B. Saunders Co., 2012.
2. A. F. Wells, Structural Inorganic Chemistry, 6th Ed; Oxford, 1987.
3. Edited by G. Wilkinson, F.G.A. Stone and E.W. Abel (9 volumes), Comprehensive Organometallic chemistry, 1982.
4. R. B. Jordan, Reaction Mechanisms of Inorganic & Organometallic systems, 2nd Ed., Oxford University Press, New York 1998.
5. G. A. Spessard & G. L. Miessler, Organometallic Chemistry, 3rd edition, Oxford University Press, 2015.

PCHM-302: Polymer Chemistry

(3 CREDITS – 42 Hours)

Course Objectives:

1. To study various methods employed in 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, 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.

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

Syllabus:

1. Step Polymerisation:

Mechanism of step polymerisation - kinetics of step polymerization	2 hours
Molecular weight control in linear polymerization	1 hour
Molecular weight distribution in linear polymerisation polyfunctional step reaction polymerisation	1 hour
Newer types of step polymerisation.	1 hour

2. Radical Chain Polymerisation:

Nature of radical chain polymerisation - Rate of radical chain polymerisation	1 hour
Initiation - molecular weight - chain transfer - inhibition and retardation	2 hours
Determination of absolute rate constants - energetic characteristics	1 hour
Auto acceleration	1 hour
General considerations on Living Radical Polymerisation	1 hour
Introduction to ATRP and RAFT	2 hours

3. Emulsion polymerisation:

Qualitative picture - quantitative aspects - other characteristics of emulsion polymerisation. 3 hours

4. Ionic chain polymerisation:

Comparison of radical and ionic polymerisations	1 hour
kinetics - cationic polymerisation of the carbon - carbon double bond	1 hour
Anionic polymerisation of the carbon - carbon double bond - Block copolymers.	1 hour

5. Chain copolymerisation:

Copolymer composition – Radical co-polymerisation - ionic co-polymerisation	1 hour
kinetics of co-polymerisation. Applications of co-polymerisation (application of polymer resins in chemical reactions)	1 hour

6. Ring opening polymerisation: General characteristics - Cyclic ethers - Cyclic amides. 1 hour

7. Stereochemistry of polymerisation:
Types of stereo isomerism in polymers - Properties of stereo regular polymers 1 hour
Forces of stereoregulations in alkene polymerisation, - kinetics 3 hours

8. 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

9. Mechanical behavior of polymers:
Mechanism of deformations and for 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

10. Polymer Characterisation:
Molecular weight: different types and their determination using end group analysis, membrane osmometry, light scattering, viscosity measurements and gel permeation chromatography
2 hours
Electron microscopy and diffraction 2 hours

11. Conducting polymers: General characteristics with examples. 1 hour

12. Polymer additives: 2 hours
Plasticizers, Antioxidants, heat stabilizers, UV Stabilizers, Flame retarders, Colorants, Curing agents and lubricants.

13. Basics of Polymer Processing: 1 hour
Extrusion, molding (compression, transfer, injection, thermoforming, blow molding, reaction injection molding), calendaring and coating.

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

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. F.W. Billmeyer, Jr., Text Book of Polymer Science, 3rd ed., John Wiley & Sons, New York 1984.
4. R.J. Young and P.A. Lovell, Introduction to Polymers, 2nd ed., Chapman & Hall, London 1991.
5. W. D. Callister Jr. and D. G. Rethwisch, Materials Science and Engineering – An Introduction, 9th edition, 2014, Wiley NJ.
6. C.E. Carraher Jr., Seymour/Carraher's Polymer Chemistry, 5th ed., Marcel Dekker Inc., New York 2000.

7. Joel R Friend, Polymer Science and Technolog, 3rd Edition, Pearson Education, New Jersey, 2014.
8.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, NewJersey 1993.

PCHM-303 E-I (i): Synthetic Organic Chemistry
ELECTIVE-I

(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. Write retrosynthetic analysis and propose a synthetic route for 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:

Johnson-Claisen Rearrangement, Eschenmoser fragmentation, Nef reaction, Bamford Stevens reaction, Peterson Olefination reaction, Tebbe Olefination reaction, Julia Olefination reaction, Nazarov Cyclization, Sharpless asymmetric dihydroxylation, Mitsunobu Reaction (Diethyl azodicarboxylate-DEAD), Tukumaya-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, Copper chromite & Wilkinsons catalyst) - Catalytic transfer hydrogenation - Problem solving -2 hours

4. 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

5. 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

6. Diastereoselectivity- Stereo selective reactions – Prochirality - Diastereoselective addition to carbonyl group without rings -2 hours

7. Asymetric 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 - organo catalysis -2 hours

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

9. 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

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

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

References:

PRESCRIBED BOOKS:

1. Raymond. K. Mackie & David M. Smith, Guidebook to Organic Synthesis, ELBS, Sec.Ed.1990.
2. J. Clayden, N. Greeves, S. Warren, P. Wothers, Organic chemistry, Oxford University Press, Sec. Ed. 2005
3. W. Carruthers, Modern Methods of Organic Synthesis, Cambridge University Press, 1987.
4. Heming Lund, Organic Electro chemistry, 2^{nd} Ed.,New York, Marcel Decker, 1983.
5. Jan Kopecky, Organic Photochemistry, VCH, 1991.
6. John Jones, The Chemical Synthesis of Peptides, Oxford University Press, 1991.
7. F. Carey and R.J. Sundberg, Advanced Organic Chemistry, Part-B, Plenum Press 2^{nd} Ed., 1984.
8. R.O.C. Norman, Principles of Organic Synthesis, 2^{nd} Ed., Chapman and Hall, 1978.
9. P.S. Kalsi, Organic reactions and mechanisms, 3^{rd} edition, New age international Publishers 2010.
10. R.O.C. Norman, Combinatorial chemistry, 2^{nd} edition, Chapman and Hall, 1978.

REFERENCE BOOKS:

1. Kurt Faber, Bio-transformations in Organic Chemistry, Springer Verlag, Berlin, 1992.
2. S. Warren, Designing organic synthesis, John Wiley Sons 1982.
3. House, Modern synthetic reactions, 2nd Ed., Benjamin Cummins Publications, 1972.
4. E.J. Corey and Xue-Min Cheng, The Logic of Chemical Synthesis, John Wiley and Sons, 1989.
5. Ed. J.D.Coyle, Photochemistry in Organic Synthesis, RSC, 1986.
6. Albert J. Fry, Synthetic Organic Electrochemistry, 2nd Ed., John Wiley and Sons, 1989.

PCHM-303 E-I (ii): Nanoscience and Nanotechnology

(3 CREDITS – 42 Hours)

Course Objectives:

1. To introduce the interdisciplinary field of nanoscience and nanotechnology to the students and to give a good overview of the field
2. To teach the principles governing the effect of size on material properties at nanoscale
3. To gain in-depth knowledge of applications of nanoscience and nanotechnology in various fields
4. To familiarize the student with various nanoscale fabrication and characterization techniques
5. To familiarize the students to the more recent areas of soft lithography, microfluidics etc
6. To create awareness of the impact of nanoscience and nanotechnology on environment and society

Course Outcomes: Upon completion the student will be able to

1. get familiarized with the basic concepts of nanoscience and nanotechnology
2. possess knowledge of different methods that can employed to fabricate matter at nanoscale
3. gain sufficient exposure to techniques used in nanoscience and nanotechnology (synthesis, fabrication, characterization) and acquire the ability to use them in solving practical problems in different sectors
4. have a good exposure to the applications of nanoscience and nanotechnology in various sectors
5. possess sufficient knowledge of soft lithography and microfluidics so as to be in a position to pursue them in the future
6. understand the impact on nanoscience and nanotechnology on environment and society

Syllabus:

1. Introduction to Nanotechnology

Introduction to Nanotechnology – The world of small dimensions -1 hour

Size dependent properties-Band Gap, Melting Point, Optical Properties, Electric Properties, Magnetic Properties; -3 hours

Classification of Nanomaterials Based on Dimensionality-0D, 1D, 2D, 3D; -1 hour

Applications of Nanotechnology in various fields. -2 hours

2. Nanofabrication - Physical, Chemical and Biological Methods

Top-Down and Bottom-Up Approaches

Solid- State Reaction Route, Kinetics of Solid State Reactions -2 hours

Mechanical Alloying; Mechanical alloying -1 hours

Soft Chemistry Routes: Solvothermal/Hydrothermal Method, Sol-Gel Method; -2 hours

Preparation of Materials in Different Configurations (Bulk, Polycrystalline, Ceramic, Single Crystals, Thin Films); -2 hours

Crystal Growth Techniques (Solid-Solid, Liquid-Solid, Gas-Solid Equilibrium): Bridgman and Stockbarger Method, Zone Melting, Flux Method; -3 hours

Thin Film Preparation: AC/DC Sputtering, Laser Ablation, Growth Kinetics, Influence of Substrate Material on The Growth Aspects of Films; -3 hours

Synthesis involving Microbes, Plant Extracts and Enzymes -1 hour

3. Engineered Nanomaterials

Metal Nanoparticles, Magnetic Nanoparticles, Quantum Dots, Nanoporous Materials (Metallic, Zeolite, MOFs) – Synthesis, Properties and Applications -2 hours

4. Nanostructure Visualization/Characterization Techniques

Electron microscopy (Cryo-SEM) -2 hours
Diffraction techniques (XRD, Synchrotron) -2 hours
Other Techniques - Concentration Determination of Nanoparticles, Zeta Potential, Absorption Spectroscopy, Static Light Scattering (SLS), Dynamic Light Scattering (DLS) -2 hours

5. Advanced Lithography Techniques:

Imprint Lithography, SPM Lithography, 3D Lithography -2 hours
Soft lithography and types - Microcontact Printing (µCP), Replica Molding (REM), Microtransfer Molding (µTM), Micromolding in Capillaries (MIMIC), Solvent-assisted Micromolding (SAMIM) -2 hours -2 hours

6. **Microfluidics and Nanofluidics**

Introduction, Basic concepts involved, Microfluidics as Technology, Application of Microfluidics and Nanofluidics in Drug Delivery, Flow Cytometry, High Throughput reactions -3 hours
Biological and Medical Microdevices: Lab on Chip, Organ-on Chip -2 hours

Surface Enhanced Raman Spectroscopy (SERS) – Principle and Applications -1 hour
Nanotechnology Safety and the Environment - Impact of Nanotechnology on Society and Industry -1 hour

References:

RECOMMENDED BOOKS:

1. Milton Ohring, Materials Science of Thin Films, II Edition, Imprint: Academic Press 2001.
2. Ben Rogers, Jesse Adams, Sumita Pennathur, Taylor and Francis Group, Nanotechnology: Understanding Small Systems, III Edition, CRC Press, 2017.
3. T. Pradeep, Nano: The Essentials, McGraw – Hill Education, 2012.
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7. Brydson, R. M.; Hammond, C., Generic Methodologies for Nanotechnology: Characterization. In *Nanoscale Science and Technology*, John Wiley & Sons, Ltd, 2005.
8. Vlassiouk, I.; Smirnov, S., Biosensing with Nanopores. In *Biosensing Using Nanomaterials*, John Wiley & Sons, Inc., 2009.
9. Marie, R.; Kristensen, A., Nanofluidic devices towards single DNA molecule sequence mapping. *Journal of Biophotonics* 2012**,** *5* (8-9), 673-686.
10. R J D Tilley, Understanding Solids: The Science of Materials, 2nd Ed., Wiley, 2013.
11. Anthony R West, Solid State Chemistry and its Applications, 2nd Ed., Wiley, 2014.
12. Sulabha K. Kulkarni, Nanotechnology: Principles and Practices, 3rd Ed., Springer 2014.

REFERENCE BOOKS:

1. Richard A.L. Jones, Soft Machines: Nanotechnology and Life, Oxford University Press, 2008.

2. Lii, J.; Hsu, W.-J.; Lee, S. P.; Sia, S. K., Microfluidics. In *Kirk-Othmer Encyclopedia of Chemical Technology*, John Wiley & Sons, Inc., 2000.
3. Gibbs, M. R. J., Nanomagnetic Materials and Devices. In *Nanoscale Science and Technology*, John Wiley & Sons, Ltd, 2005.
4. Renaud, L., Microfluidics: Manipulation of Nanovolume Samples. In *Chemical Sensors and Biosensors*, John Wiley & Sons, Inc., 2012.
5. Dong, H.; Hu, W., Organic Nanomaterials. In *Springer Handbook of Nanomaterials*, Vajtai, R., Ed. Springer Berlin Heidelberg, 2013.

PCHM-304 E-II (i): Theory and Applications of Physical Methods in Chemistry
(Interdepartmental Elective)

(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. Predict the expected spectral data and/or sketch the spectrum for a given compound.

Syllabus:

Applications in Organic Chemistry and Biochemistry.

1. Use of shift reagents – in U.V. spectral analysis, with examples chosen from chemistry of naturally occurring flavonoids- where such methods have been particularly successful. -1 hour

2. I.R. spectra with regards to study of hydrogen bonding
and resonance effects in organic compounds – -1 hour

3.Advanced aspects of NMR:
Use of paramagnetic shift reagents – -1 hour
NOE effect, FT NMR its advantage- -1hour
Double resonance, with particular reference to spin - spin decouplings, solvent effects in PMR spectra -2 hours
13C NMR – Introduction and theory – -1 hour
Applications – -1 hour

4. Mass spectrometry: High resolution mass spectral fragmentation mechanism, soft ionization techniques. -1 hour

5. Combined problem solving: extensive analysis of problems based on integrated spectral data with examples chosen from natural products -3 hours.

6. Two dimensional NMR spectroscopy:
Introduction - Theory and applications of DEPT spectra and Homo COSY – -2 hours
Applications of Hetro COSY- HMQC and HSQC -2 hours
Incredible natural abundance double quantum transfer experiment (2-D INADEQUATE) - Problem solving. -2 hours

7. CD technique for Biology samples: CD of proteins, peptide conformations, DNA-protein and protein-protein interactions. -2 hours

Theoretical principles and Applications in Inorganic chemistry.

8. Introduction: A brief review of the selection rules for absorption of radiation by molecular vibrations, Intensity and line width of spectral line. Population of various states and intensity. Doppler broadening and life time broadening, factors affecting coupling, degeneracy. -2 hours

9. 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 co-ordination on spectra due to change in symmetry – -1 hour

10. 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 - poly atomic molecules - linear, symmetric top and asymmetric top molecules (only spectral features) – -2 hours
Basic outline of the instrumentation of microwave technique- -1 hour

11.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 CO_2, N_2O, SO_2, NO_3^-, ClO_3^- and ClF_3 using Raman spectroscopy – -1 hour
Basic instrumentation – -1 hour

12. 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

13. Electron paramagnetic resonance: Theory and applications to Nickel(II) & Copper(II) compounds, magnetic exchange process in dinuclear complexes - -2 hours.

14. Mossbauer spectroscopy: Origin and interpretation of Mossbauer effect-
Mossbauer chemical shift -1 hour
Application of Mossbauer spectroscopy to Fe and Sn systems -1 hour

References:

PRESCRIBED BOOKS:

1. Pavia, Lampman and Kriz, Introduction to Spectroscopy, A Guide to students of Organic Chemistry, 5th Ed, 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.
4. C.N. Banwell, Fundamentals of Molecular Spectroscopy, 3rd Ed., T.M.H. Publishing Co 1980.
5. R.S. Drago, Physical Methods in Inorganic Chemistry, East - West Press 1968.
6. E.A.V. Ebsworth, Structural Methods in Inorganic chemistry, 2nd Ed. D.W.H. Rankin and S. Cradock, 1991.
7. Nakanishi and Solomon, IR Spectroscopy, 2nd Ed, Holden Day 1977.
8. Laszolo and Stale, Organic Spectroscopy - Principles and applications, Harper and Row1971.
9. Kensl E. Van Holde, W. Curtis Johnson, P. Shing Ho, Principles of Physical Biochemistry, 2nd Ed., Pearson Prentice Hall, 2005.
10. Cantor and Schimmel, Biophysical chemistry Part II: Techniques for the Study of Biological Structure and Function, 10th Ed., W. H. Freeman and Company, 1980.

REFERENCE BOOKS:

1. G.M. Barrow, Introduction to Molecular Spectroscopy, McGraw - Hill 1962.
2. J. Devis and C.H.J. Well, Spectral problems in Organic Chemistry, Chapman and Hall 1984.
3. P. Lazalo, NMR of newly accessible nuclei, Vols: 1&2, Academic Press 1983.
4. J.W. Akitt, NMR and Chemistry, 2^{nd} Ed., Chapman and Hall 1984.
5. Levy, Lichter and Nelson, Carbon -13 NMR spectroscopy, 2^{nd} Ed., Chapman and Hall 1980.

PCHM-304 E-II (ii): Materials And Their Characterization
(3 CREDITS – 42 Hours)
Course Objectives:
1. To understand various classes of materials, and their structural characteristics
2. To gain an understanding of techniques that are used for structural and surface characterization of materials
Course Outcomes: Upon completion the student will be able to
1. Identify various classes of materials and their properties
2. Analyze materials properties using appropriate characterization techniques
3. Solve numerical problems related to systems studied
Syllabus:

1. Materials classification:

Based on (a) crystallinity: Amorphous, polycrystalline and single crystalline materials — 2 hours
Based on (b) physical properties - includes metals, semiconductors, insulators, glasses — 2 hours

2. Introduction to Crystallography:

Crystal lattices, crystal structures and crystal systems — 1 hour
Crystal planes and Miller indices (cubic and hexagonal crystals), crystal directions — 2 hours
Introduction to reciprocal lattice; Ewald Sphere and Derivation of Bragg's law — 2 hours

3. Introduction to defects:

Point defects in crystal elements, solid solutions, Schottky defects, Frenkel Defects, Non-stoichiometric compounds — 1 hour
Linear defects: Edge dislocation, screw dislocation, partial and mixed dislocations — 2 hours
Planar defects:
external surfaces, grain boundaries, phase boundaries, twin boundaries, antiphase boundaries — 2 hours
Volume defects: precipitates — 1 hour

4. Electron spectroscopy- X-ray photoelectron spectroscopy and UV Photoelectron spectroscopy:

Introduction - experimental aspects of PES, instrumentation — 1 hour
Ionisation energies Core electron PES: X- PES (ESCA) elemental analysis — 1 hour
Chemical shift in X-PES - spin orbital coupling in PES — 1 hour

5. Diffraction methods:

Powder X-ray diffraction – compound identification, lattice parameter — 3 hours
Crystallite size effect — 1 hour
Lattice strain measurements; single crystal X-ray diffraction — 1 hour
Electron diffraction. — 1 hour

6. Light Microscopy methods:

Optical principles and instrumentation — 2 hours
Specimen preparation, and imaging modes — 2 hours
Phase contrast microscopy, and confocal microscopy — 2 hours

7. Electron Microscopy methods:	
Scanning electron microscopy: instrumentation, principles and applications	2 hours
Transmission electron microscopy: instrumentation, principles and applications	2 hours
Energy-dispersive X-ray spectroscopy	1 hour
8. Scanning probe microscopy:	
Scanning tunneling microscopy	2 hours
Atomic force microscopy and various modes	2 hours
9. Thermal analysis methods (instrumentation and applications):	
Thermogravimetric analysis and differential thermal analysis: applications to study of materials	2 hours
Differential scanning calorimetry: applications to study of materials	1 hour

References:

PRESCRIBED BOOKS:

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. W. D. Callister, Materials Science and Engineering, Wiley, 2010.
5. Anthony R West, Solid State Chemistry and its Applications, Wiley, 2014.
6. Yang Leng, Materials Characterization: Introduction to Microscopic and Spectroscopic Methods, John Wiley & Sons (Asia) Pte Ltd, (2008).
7. B. D. Cullity and S. R. Stock, Elements of X-ray Diffraction, 3rd ed., Prentice Hall, (2014).
8. David B. Williams and Barry C. Carter, Transmission Electron Microscopy: A text book for Materials Science, Springer, (2009).
9. Sam Zhang, Lin Li, Ashok Kumar, Materials Characterization Techniques, CRC Press (2009)
10. Stefan Hufner, Photoelectron Spectroscopy – Principles and Applications, 3rd edition, Springer-Verlag GmbH 2003
11. Hour 20 Photoelectron spectroscopy in Physical Methods and Molecule Structure 2, 2nd ed.; As part of series Science: A third Level Course - The Nature of Chemistry, The Open University Press, Milton Keynes 1980.
12. Photoelectron and Auger Spectroscopy by Thomas A Carlson, Plenum Press, 1975.
13. Douglas A. Skoog, F. James Holler, Stanley R. Crouch, Principles of Instrumental Analysis, 7th ed., Cengage Learning 2018

PPHY-EL12: Biomaterials (Interdepartmental elective)
(3 credits – 42 hours)
The title of the paper and the syllabus are same as the elective paper offered by the Department of Physics, SSSIHL

PCHM-305: Computational Applications in Chemistry – I

2 CREDITS

Course Objectives:

1. Introduce Python programming to students
2. To introduce the fundamental concepts of molecular modelling and simulation to students
3. To motivate/train students to apply these concepts/techniques to solve interesting research problems.

Course Outcomes: Upon completion the student will be able to

1. Gain hands-on experience in drawing structures using Hyperchem and other software
2. Perform computational calculations using Gaussian and Hyperchem
3. Explore drug design using docking studies
4. Use molecular modelling software to study reaction mechanisms

Syllabus:

Introduction to Molecular Modeling; MO Theory: Ab Initio From the Beginning.	
Potential Energy Surfaces & Optimization Methods;	4 hours
Introduction to Python	3 hours
Methods for Electron Correlation; Semi-Empirical Molecular Orbital Methods	4 hours
Density Functional Theory (DFT);	3 hours
Introduction to Hyperchemlite, Gaussian, Autodock, MOE	4 hours
Various applications of the above levels to organic reactions (like conformational analysis)	
Lab problem	4 hours
Studying reaction pathways using Intrinsic reaction coordinate method	
Reaction Dynamics: Calculating Potential Energy Diagram of Br. + Br_2 reaction	2 hours
Natural Bond Orbital and Atoms in Molecule analyses	1 hour
Calculating the Thermodynamic Properties, HOMO, LUMO, Ionization Potentials,	
Chemical Hardness, Softness, Dipole Moment, Polarizability	2 hours
Data Science & Data Mining in Material Science	1 hour

References:

1. David C. Young, Computational Chemistry: A Practical Guide for Applying Techniques to Real-World Problems. John Wiley & Sons, Inc. 2011.
2. Computational Chemistry of Solid State Materials -A Guide for Materials Scientists, Chemists, Physicists and others by Richard Dronskowski, WILEY-VCH Verlag GmbH & Co. KGaA. 2008.
3. A Chemist's Guide to Density Functional Theory - Koch, W., Holthausen, M. C. 3rd Ed., ISBN 3-527-30372-3. 2004.
4. Essentials of Computational Chemistry Theories and Models, Cramer, C. J. 2nd Ed., ISBN 0-470-09182-7. 2013.

PCHM-306: Project work (Interim Review)
At the end of the third semester assessment of the project work will be done along with the literature review.

PCHM-401: Solid State Chemistry and Nanomaterials
(2 CREDITS – 28 Hours)
Course Objectives:
1. This unique and popular course satisfies SSSIHL's general chemistry degree requirement, with an emphasis on solid-state materials and their properties.
2. To provide an introduction to the concepts underlying solid state chemistry
3. To illustrate the wide range of materials and physical properties that are currently available
Course Outcomes: Upon completion the student will be able to 1. To get an overview of solid state synthesis and properties of inorganic materials. 2. To give an account of the generation of X-ray radiation and its effects on matter 3. To be able to synthesize carbon nanomaterials
Syllabus:
Preparative methods: Solid state reactions general principles, experimental procedure, -1 hour Co-precipitation as a precursor to solid state reactions, -1hour Kinetics of solid state reactions- -1hour Crystallizations of solutions, melts, glasses and gels, vapour phase transport methods, ion exchange reactions, electro chemical reduction methods and thin film preparation, growth of single crystals -2 hours **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 **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 **Electrical properties**- Hall effect, dielectric materials, ferro-pyro-piezo electricity and its applications-1 hour **Magnetic properties:** Classification of materials -Dia, para, ferro, ferri, and antiferro magnetic types-2 hours Selected magnetic materials such as spinels, garnets and perovskites- -1 hour **Superconductivity:** Theory, discovery and recent high Tc materials -2 hours **Organic solids state chemistry**-Topochemical control of organic solid state reactions Electrically conducting solids, organic charge transfer complex, organic metals, new super conductors -2 hours **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, W. S. E. Wiley, 2003.
2. Poole and Owens, Introduction to Nanotechnology Wiley, 2003
3. L. Smart and E. Moore, Solid State Chemistry, Chapmann 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.

PCHM-402: Supramolecular Chemistry

(2 CREDITS – 28 Hours)

Course Objectives:

1. To discuss concepts central to non-covalent interactions and host-guest interactions
2. To discuss manifestation of supramolecular self-assembly in biological and synthetic systems

Course Outcomes: Upon completion the student will be able to

1. Appreciate role of supramolecular interactions 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 nano-biotechnology; 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.

SUGGESTED READING:

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 a brief outline involved in the process of drug design and to understand the basic aspects related to it.
2. To give an understanding of chemistry of some essential vitamins and antibiotics.
3. To highlight the importance of drugs from natural products with special reference to medicinal plants of Indian and Chinese origin.
4. To understand basic aspects related to polymer stability and polymer degradation in the environment.

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. Apply methodologies learnt to tackle simple research problems.

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 -1hour
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 Hyperchem lite and Autodoc to get hands on experience) -1hour

2. Pharmacokinetics & Pharmacodynamics:

Introduction of drug absorption, bioavailability (factors effecting 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 -1hour

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. M.E. Wolff, (Editor) Burger's Medicinal chemistry, Volume I, 5th Ed, John Wiley & Sons, 1995.
2. N.O. Foye, Lea and Febiger (Editors)Principles of Medicinal Chemistry, Philadelphia, 1976.
3. C. Hansch, P.G. Sammes and J. B. Taylor(Editors) Comprehensive Medicinal Chemistry Vol 4 , Quantitative Drug Design, Pergamon Press, 1990.
4. Molecular Recognition of Amiloride Analogs: A Molecular Electrostatic Potential Analysis, J. Med. Chem., 35, p 1643, 1992.
5. Robert K. Murry, D.K. Granner, P.A. Mayes and V.W. Rodwell Harper's Biochemistry, 25th Ed. Mc Graw 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, Volkhard Sustel(Editors), Modern Drug Research, Vol.12, Paths to better and safer drugs, Marcel Dekker. Inc, 1989.
3. Kirk Othmer's Encyclopaedia of Chemical Technology 3rd edition, Wiley Interscience Publication. 1978 - 84
4. Ullmann's Encyclopaedia of Industrial Chemistry VCH Publishers, Wurz Burg, Federal Republic of Germany, 1987-89.
5. Remington's Practice of Pharmacy, 13th Ed., The Mach Publishing Company, Eastern P.A. 1979.

PCHM-404 E-III (i): Environmental Chemistry
(Interdepartmental 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, waste water 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 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. Should acquire the ability to apply the concepts studied in the course for solving environmental problems
3. Student should understand the need to live in harmony with nature.

Syllabus:

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 hour

Particles in the atmosphere - physical behavior - physical and chemical processes for particle formation -1 hour

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

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

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 -1hour
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

Oils in Fresh & Marine Water:
Sources of oil pollution -Chemistry and fate of hydrocarbons –
Oil in run off and ground water – -1 hour
Biodegradation - effect on aquatic organisms and commhouries – -1 hour
Treatment and disposal technology. -1 hour

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

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 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

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 Fresh Water, Pergamon, 1987.
3. Lippmann and Schlesinger, Chemical Contamination in the Human Environment, OUP, Oxford, 1979.
4. H.M. Dix, Environmental Pollution, Wiley, 1981.
5. A.K. De, Environmental Chemistry, 2nd Ed., Wiley Eastern 1989.
6. J.M. Montgomery, Water Treatment - Principles and Design, Wiley, 1985.

7. R.M. Harrison Pollution: Causes, Effects and Control, 3rd Ed., Royal Society of Chemistry, London, 1996.

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-III (ii) Advanced Aspects of Applications of Group Theory in Chemistry (Interdepartmental Elective)

(3 CREDITS – 42 Hours)

Course Objectives:

1. To understand the molecular symmetry operations and classification of molecules into different point groups.
2. To derive selection rules for IR and Raman activity using group theory
3. To construct molecular orbitals of metal complexes with ligands of different types.
4. To get free ion configurations terms and states, and LFT of coordination compounds.
5. To understand the origin of bands in the electronic spectra of coordination compounds and evaluation of Racah parameters.

Course Outcomes: Upon completion the student will be able to

1. classify molecules into different point groups and construct their character table.
2. compare compounds of different chemical behaviour under the same point group.
3. draw molecular orbital diagrams of metal complexes
4. Understanding LFT theory and origin of electronic transitions to explain the spectra of coordination compounds.
5. explain Orgel and Tanabe-Sugano diagrams.

Syllabus:

Concept of symmetry in molecules: symmetry elements, Cartesian coordinate system and symmetry elements -more about symmetry elements, -1 hour
mathematical requirements for a point group. -1 hour
Molecular point groups: molecules of low symmetry and high symmetry, molecules of special symmetry-notation of point groups-descent in symmetry in molecules with substitution -3 hours
Symmetry criteria for optical activity-symmetry restrictions on dipole moments and stereo isomerism. -2 hours

Infra-red and Raman spectroscopy of molecules: symmetry based selection rules of IR, Raman,-symmetry requirements for overtones, binary and ternary combination bands, Fermi resonance. -3 hours

Molecular orbital theory of metal complexes: linear combination of atomic orbitals theory-MO energy level diagram for a diatomic molecules- -3 hours
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, MO theory of sandwich complexes -3 hours

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- -3 hours
Molecular term symbols derivation notation and selection rules for transition -2 hours

Ligand field theory of coordination compounds: simple crystal field theory of ML_5 complexes, effect of weak crystal field on terms, ligand field term diagrams, -3 hours

Orgel diagrams, correlation diagrams, -3 hours s
Tanabe-Sugano diagrams of different d-orbital configurations -3 hours

Electronic spectra of metal complexes: selection rules for electronic spectra-electric dipole transitions, magnetic dipole transitions, nature of electronic spectral bands, -3 hours
classification of electronic spectra, charge transfer spectra, -2 hours
evolution of Dq, B' and β parameters, graphical method, Konigs numerical method electronic spectra of lanthanides and actinides. -2 hours

References:

PRESCRIBED BOOKS:

1. K. Veera Reddy, Symmetry and spectroscopy of molecules, New age international (P) ltd, publishers Second revised edition 2009
2. ABP. Lever, Inorganic electron spectroscopy, Second edition Elsevier Amsterdam(1984)
3. G Wilkinson. Rd Gillard and JaMc Cleverty (Editors)Comprehensive coordination chemistry, Volumes 1-7 Pergamon press, New York 1987
4. B.N.Figgis and M.A. Hitchman ,Ligand field theory and its applications, Wiley-VCH, 2000
5. F.A. Cotton, Chemical Applications of Group Theory, 3rd Ed., Wiley ,1990
6. P.W.Atkins, T.L. Overton, J.P. Rourke, M.T. Weller, and F.A. Armstrong,
7. Shriver & Atkins' Inorganic Chemistry, Fifth edition, W.H.Freeman and company, 2010

REFERENCE BOOKS:

1. N B Colthup, LH Daly and S E Wiberley Introduction to infrared and Raman spectroscopy, Second edition, Academic Press, New York(1975)
2. A. Streitweiser, Jr., Molecular orbital theory for organic chemists, John Wiley & Sons Inc., New York (1961)
3. I. Hargittai and M. Hargittai Symmetry through the eyes of a chemist, , Verlagsgesellschaft, Germany(1986).
4. H H Jaffe and M Orchin Theory and applications of UV spectroscopy,
   Wiley New York 1962
5. M.Orchin, H H Jaffe ,Symmetry orbitals and spectra,
   Symmetry orbitals and spectra, Wiley (inter science) New York 1970

PBIO-404 E-IV (BT-4): Environmental Biotechnology (Inter-departmental Elective)

(3 CREDITS – 42 Hours)

The title of the paper and the syllabus are same as the elective paper offered by the Department of Biosciences, SSSIHL

PCHM-405 E-IV (i): Biocatalysis for Industry and Environment
(Inter Departmental Elective)

(3 CREDITS – 42 Hours)

Course Objectives:

1. To study the advantages and limitations of using biocatalysts for synthesis, and the criteria that one may choose for using these over inorganic catalysts
2. To provide an overview of the different enzyme classes coupled to the catalyzed chemical reactions and describe stereochemistry and methods to optimize the stereochemical outcome.
3. To introduce the concepts of bioreactor configurations and operation
4. To discuss several industrial processes as examples.

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 decide which chemical reactions can enzymes from a certain class exhibit.
2. recognize advantages and disadvantages of different reaction media for enzymatic reactions and be able to decide suitable reaction conditions in individual cases.
3. decide on the type of reactor configuration needed based on the transformations that need to be carried out.
4. understand the largescale bioremediation techniques employed.

Syllabus:

Bio transformation, 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 hour
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 Bio-transformations 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

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
noncompetitive/uncompetitive inhibition, irreversible inhibition. -2 hours
pH effects on enzyme kinetics . -1 hour

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, hydro-xylation of steroids at unactivated carbon centers, Case Study. -2 hours

Bioremediation and Biological Method 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 pcb's. -1 hour

Anaerobic and aerobic degradation, site characterization, treatability assessment, remediation technology selection -2 hours

Design of in situ remediation techniques, phyto remediations, 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 ,Bio-transformations in Organic Chemistry , Springer Verlag, Berlin, 1992.
5. Pauline M. Doran ,Bioprocess Engineering Principles, Academic Press. 1995, ISBN-13:978-0-12-220856-0
6. Michael L. Shuler and Fikret Kargi Bioprocess Engineering, Basic concepts , Second Edition, PTR Prentice Hall. 2001, ISBN 0-13-081908-5.
7. Peter Grunwald ,Biocatalysis: Biochemical fundamentals and applications , Imperial college Press,2009, ISBN-13 978-1-86094-771-1; ISBN-10 1-86094-771-9
8. Gideon Grogan ,Practical Biotransformations: A beginners' guide , First edition, John Wiley & Sons,2009, ISBN 9781405193672.

REFERENCE BOOKS:

1. Nicholas K. Terrett Combinatorial Chemistry,Oxford Chemistry Masters, Oxford University Press, 1988.
2. S. Warren ,Designing organic synthesis , John Wiley Sons 1982.
3. E.J. Corey and Xue-Min Cheng ,The Logic of Chemical Synthesis , John Wiley and Sons, 1989.

PCHM-405 E-IV (ii) Organic Chemistry of Natural Products	
	(3 CREDITS – 42 Hours)
Course Objectives:	
1. To provide an overview of the field of natural product chemistry	
2. Using the selected examples, this course describes the process of identification and isolation of natural products from natural sources,	
3. The course covers their chemical synthesis, biological activities, ecological relevance	
4. Special emphasis will be given to secondary metabolites isolated from terpenes, alkaloids and flavonoids	
5. To learn organic chemistry through natural products	
Course Outcomes: Upon completion the student will be able to	
1. predict the biosynthetic pathways of a secondary metabolite	
2. outline total synthesis of new metabolites	
3. isolate, purify and characterize secondary metabolite structures	
4. solve organic chemistry problems using biological properties and spectral methods	
Syllabus:	
Methods in Natural Product Chemistry: Techniques used in isolation	-1 hour
Determination of structures of different types of plant secondary metabolites-	-2 hours
Biosynthesis - a brief introduction to acetate malonate pathway	-1 hour
Acetate mevalonate pathway	-2 hours
Shikimic acid pathway	-2 hours
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
Alkaloids:	
Biosynthesis of opium alkaloids: Stereochemistry and rearrangements of morphine	-2 hours
Determination of structure of strychnine and its total synthesis	-2 hours
Stereochemistry and synthesis of quinine –	-2 hours
Photochemistry of Colchicine-	-2 hours
Oxygen Heterocyclic Compounds: Structure elucidation of flavonoids with a suitable example (use of colour reactions, UV, MS,13C&1H NMR)-	-2 hours
Determination of structure of scandenin by spectral methods	-2 hours.
Antibiotics: Reactions & synthesis of penicillin	-2hours
Total synthesis of anti-cancer antibiotics such as daunorubicin	-3 hours
Chemical Ecology: An introductory study:	
chemistry of insects with particular reference to chemical defense mechanisms, pheromones	-2 hours

Plant defense chemicals - Allelo - chemicals and Phytoalexins –
(examples and their use in agriculture) -2 hours

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. Nakanishi et al (Editors)Natural Products , Vols 1, 2 and 3, Academic press 1974, 1975 and 1983.
3. K. C. Nicolaou and E. J. Sorensen ,Classics in Total Syntheses , VCH, 1996.
4. J. Mann, R. S. Davidson, J. B. Hobbs, D. V. Banthorpe and J. B. Harborne ,Natural Products, Addison Wesley Longman Limited, 1994.

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. Barton Oilis (Editor),Comprehensive Organic Chemistry Ed,. by Barton Oilis, Vol 5, Biological compounds, Pergamon press, 1979.
3. J.Apsimon (Editor),Total synthesis of Natural products, Vols I,V and VI Academic Press, 1973, 1983 and 1984,

PPHY-EL21: Graphene and 2-dimensional Materials (Interdepartmental elective)
(3 credits – 42 hours)
The title of the paper and the syllabus are same as the elective paper offered by the Department of Physics, SSSIHL

PCHM-406: Computational Applications in Chemistry – II

2 CREDITS

Course Objectives:

1. To introduce the concept of molecular dynamics (MD)
2. To understand the quantum mechanical aspects of molecular modelling

Course Outcomes: Upon completion the student will be able to

1. Perform molecular dynamic simulations
2. Run GROMACS and compute various properties of macromolecular systems
3. Evaluate theoretically the effect of solvents on drug interactions using dynamics

Syllabus:

Introduction to Molecular Mechanics	2 hours
Introduction to various force fields	2 hours
Force field parameterization	2 hours
Basics of Molecular Dynamics Simulation	2 hours
Setting up of the MD simulations and running the minimization,2 hours	
Optimization and trajectory generation	4 hours
Using Molecular Dynamics to Compute Properties	6 hours
Introduction to Gromacs	6 hours
Electrostatics & Solvation in Biomolecules	2 hours
Calculation of Free Energy	1 hour
Quantum Mechanics/Molecular Mechanics (QM/MM)	1 hour

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.

PCHM-407: Project work –II

8 CREDITS

Submission of dissertation and comprehensive viva of the project work

Dept. of Physics – M.Sc.

PPHY-EL 12: Biomaterials

(3 CREDITS – 42 Hours)

Course Objectives:

To introduce various types of biomaterials, their properties and medical applications.

Course Outcome: Upon completion the student will

Learn about different types of biomaterials, their mechanical properties, selection of biomaterials for different applications, toxicity and corrosion related issues.

Syllabus:

1. **Definitions:** Biomaterials, Biomedical materials and Biological materials, Biocompatibility *2 hrs*

2. **Toxicity and corrosion:** Elements in the body, Biological roles and Toxicities of trace elements, Selection of metallic elements in Medical-Grade alloys, Corrosion of Metals, Environment inside the Body, Minimization of Toxicity of Metal Implants, Biological Roles of Alloying Elements. 9 *hrs*

3. **Mechanical Properties of Biomaterials:** Role of Implant Biomaterials, Mechanical Properties of General Importance - Hardness, Resilience and Strechability, Failure, Essential Mechanical Properties of Orthopedic Implant Biomaterials. 9 *hrs*

4. **Metallic Biomaterials:** Development of Metallic Biomaterials, Stainless Steels, Cobalt-Based Alloys, Titanium Alloys, Comparison of Stainless Steels, Cobalt, and Titanium Alloys, Dental Materials, Ni-Ti Shape-Memory Alloys; Other Clinically Applied Metallic Materials, New Metallic Materials: Magnesium Alloys. *8 hrs*

5. **Bioinert Ceramics:** Overview of Bioceramics, Inert Bioceramics: Al_2O_3, ZrO_2, Types of Joints, Total Joint Replacement. *7 hrs*

6. Biomaterials for dental applications; Polymeric Biomaterials and Bioinert Polymers. *7 hrs*

References:

1. Larry L Hench, An Introduction to Bioceramics: Second Edition, Imperial College Press, 2013.
2. Qizhi Chen, George Thouas, Biomaterials: A Basic Introduction, CRC Press, 2014.
3. David Williams, Essential Biomaterials Science, Cambridge University Press, 2014.
4. Joon Park, Bioceramics: Properties, characterizations, and applications, Springer, 2008.

Dept. of Physics – M.Sc.

PPHY-EL 21: Graphene and 2-Dimensional Materials

(3 CREDITS – 42 Hours)

Course Objectives:

This course deals with physics and applications of devices based on graphene and other two dimensional materials such as MoS_2

Course Outcomes: Upon completion the student will be able to

acquire knowledge of various synthesis routes for making graphene and some other 2D materials; understand Raman spectral signatures of these 2D materials; understand some mechanical and chemical properties; and their applications.

Syllabus:

1. **Introduction:** History of graphene, Atomic structure and graphene, Imaging the structure of graphene, Properties of graphene overview *2 hrs*

2. **Production of graphene and 2-d materials:** Comparison of production methods, Scotch-tape method (micromechanical cleavage), Chemical vapour deposition, Solution-exfoliation – graphene and other 2-d materials, graphene oxide, Decomposition of silicon carbide, Production of graphene nano-ribbons . *4 hrs*

3. **Electronic properties and devices:** Electronic structure of graphene, First graphene device, Further graphene devices and evidence of 2-dimensional nature, Electronic properties of bilayer graphene, Switching graphene OFF. *8 hrs*

4. **Raman spectroscopy:** Principles of Raman spectroscopy, Raman spectrum of graphene, Analysis of graphene Raman spectra, Raman spectra of other 2-D materials. *5 hrs*

5. **Chemical properties and sensors:** X-ray photoemission spectroscopy, Optical absorption spectroscopy, Functionalizing graphene, Hydrogels and aerogels, Liquid cystals, Gas and chemical sensors. *6 hrs*

6. **Mechanical properties and applications:** Measuring mechanical properties, Graphene resonators, Electromechanical devices, Graphene bubbles, Graphene composites. *5 hrs*

7. **Graphene membranes:** GO and rGO membranes, Membranes for separation, Membranes as barriers, Porous membranes, Supercapacitor electrodes. *6 hrs*

8. **Biomedical devices and 2-d heterostructures:** Biocompatibility and biodistribution, Scaffolds for tissue engineering, Drug and gene delivery, Cancer therapy, Introduction to 2-D heterostructures, 2-D heterostructure devices *6 hrs*

References:

1. Mikhail I. Katsnelson, Graphene: Carbon in Two Dimensions, Cambridge University Press, 2012.
2. Dragoman, Mircea, Dragoman, Daniela, 2D Nanoelectronics: Physics and Devices of Atomically Thin Materials, Springer, 2017.

Dept. of Biosciences – M.Sc.

PBIO-404 E-IV (BT-4): Environmental Biotechnology

(3 CREDITS – 42 Hours)

Course objective:
This course deals with biotechnological approaches for solving environmental problems.

Course outcomes:
Upon completion of the course the student will be familiar with biotechnological methods for abatement of pollution and for development of sustainable, environmentally friendly resources such as biofuels and biopesticides.

Syllabus:

1. **Natural resource management:** Types of Natural resources: Conservation and management - soil, water, minerals. forests, wildlife, energy**. 4hrs**
2. **Sources of major environmental pollutants**: Point source and non-point source; Air, water, soil and solid waste pollutants. **3hrs**
3. **Biotechnology for Pollution Abatement:** Air pollution and its control through Biotechnology. 3hrs
4. Water pollution and its control: Waste Water Treatment — Aerobic and anaerobic processes. Solid waste and soil pollution management. **5hrs**
5. **Industrial problems and their remedial mechanisms:** Pulp and Paper, Dairy, Distillery, Tannery, Sugar, Petroleum, Antibiotic industries. **5hrs**
6. **Biodegradation and conversion:** biodegradation of xenobiotic compounds and hazardous wastes: TNT wastes. dyestuff wastes, pesticides and oil-spills**. 4hrs**
7. **Eco-friendly processes for sustainable environment:**
   a. Modern fuels and their environmental impacts: Bio-methanation, Bioenergy, bioethanol and biodiesel- types of biofuels. **4hrs**
   b. Bio-pesticides and Bio-fertilizers: Thuringiensis toxin as natural pesticide. Algal, Fungal and Bacterial bio-fertilisers, composting, biopolymers and bioplastics**. 4hrs**
8. **Global environmental problems:** Deforestation and loss of biodiversity, ozone depletion, green-house effect, global warming, acid rain, biotechnological approaches for management, Pollution control measures in India. **3hrs**
9. **Bio-mineralisation:** Significance and limitations. Microorganisms involved in Bioleaching of Ores, Mechanism and Biochemical reactions involved in Bioleaching, metal recovery. **4hrs**

Basic Texts:

1. Thakur. I. S. (201 1), Environmental Biotechnology: Basic Concepts and Applications. I.K. International Publishing House Pvt Limited.
2. Agarwal, S. K. (2005). Advanced Environmental Biotechnology, APH Publishing Corporation.
3. Chatterji A. K. (2002). Introduction to Environmental Biotechnology, Prentice Hall of India Pvt Ltd.
4. Scragg. A. (1999). Environmental Biotechnology, Pearson Education Limited.
5. Srivastava, A. K., & Sohal. H. S. (1994). Environment and biotechnology. Published by S. B. Nangia for Ashish Publishing House.

Additional reading:

1. Mohapatra P.K. (2006). Textbook of Environmental Biotechnology, I.K. International Publishing House Pvt Ltd.
2. Miller. G., & Spoolman. S. (2011), Living in the Environrnent: Principles, Connections, and Solutions. Cengage Learning.
3. Chopra. V. L., Malik, V. S., & Bhat, S. R. (1999), Applied Plant Biotechnology. Science Publishers.