M. Sc.
Curriculum

Effective from July 2017 Batch

Department of Chemistry
Indian Institute of Technology Madras

July 2017

Content

A NOTE FROM THE CURRICULUM COMMITTEE

Dear Students:

Greetings!

Congratulations for achieving selection in the top higher education institute in India. We, faculty and staff of the department, heartily welcome you to Department of Chemistry, IIT Madras!

We have high expectations on your academic performance. We are sure that you will be our ‘ambassadors’ in future who will go around the world and make us proud through your excellent work.

The booklet describes the new curriculum for the M. Sc. program. Curriculum revision was a huge exercise and the committee believes that we have taken care of every aspect to arrive at comprehensive syllabus for all the courses. We take this opportunity to profusely thank all the faculty colleagues of the department for their timely suggestions, interventions and participation in the brain-storming sessions during the curriculum revision.

Wishing you an academically fruitful stay at IIT Madras!

Curriculum Committee-2017

Indrapal Singh Aidhen-Chairman

Members: S. Sankararaman, K. Mangala Sunder, Dillip K Chand and Edamana Prasad

CREDIT STRUCTURE

Semester I	Credit	Semester II	Credit	Semester III	Credit	Semester IV	Credit
CY5011 Transition Metal & Bioinorganic Chemistry	9	CY5012 Main Group Chemistry and Spectroscopic Characterization of Inorganic Compounds	9	CY6011 Solid State Chemistry	9	Elective-1	9
CY5013 Conceptual Organic Chemistry	9	CY5014 Reactive Intermediates and Concerted Reactions	9	CY6013 Spectroscopic Applications in Organic Chemistry	9	Elective-2	9
CY5015 Classical and Statistical Thermodynamics	9	CY5016 Kinetics and Reaction Dynamics	9	CY6015 Electrochemistry: Fundamentals and Applications	9	Elective-3	9
CY5017 Principles of Quantum Mechanics	10	CY5018 Chemical Bonding and Group Theory	9	CY6017 Optical and Magnetic Resonance Spectroscopy	9	Project CY6026 Or Electives 4, 5, 6	18 Or 27
CY5019 Organometallic Chemistry	9	CY5020 Analytical Chemistry: Principles, Practices and Applications	9	CY6019 (E) Modern Synthetic Methods in Organic Chemistry or CY6023 (E) New Methods and Strategies in Organic Synthesis	9		
CY5021- Introductory Computational Chemistry Laboratory	5	CY5022- Inorganic Chemistry Laboratory	5	CY6025 Project	9		
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SEMESTER-WISE CORE COURSES

CY5011: Transition Metal and Bioinorganic Chemistry

Class Hours	Expected Learning Hours by Students Outside the Class Hours	Total Credit
3	6	9

Course Objectives: The learners should be able to apply theories of chemical bonding, reaction mechanism, electronic structure and magnetic properties of coordination complexes to identify the occurrence, active site structure and functions of some transition metal ion containing metalloproteins or enzymes.

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

Identify the principles, structure and reactivity of selected coordination complexes

Interpret their electronic spectra and magnetic properties.

Utilize the principles of transition metal coordination complexes in understanding functions of biological systems.

Course Contents:

Transition Metal Chemistry: Structure, bonding and properties of transition metal ligand complexes – ligand, coordination, geometry, coordination number, isomerism (recapitulation) and optical isomerism, HSAB concept, thermodynamic stability, successive and overall stability constants, Irving-William series, chelate and macrocyclic effect.

Theories of bonding - VBT, CFT and their limitations; d-orbital splitting in octahedral, JT-distorted octahedral, square planar, square pyramidal, trigonal bipyramidal, and tetrahedral complexes; CFSE for d1 to d10 systems, pairing energy, low-spin and high-spin complexes and magnetic properties; LFT, and molecular orbital (MO) theory of selected octahedral and tetrahedral complexes.

Electronic Spectra - UV-Vis, charge transfer, colors, intensities and origin of transitions, interpretation, term symbols and splitting of terms in free atoms, selection rules for electronic transitions, Orgel and Tanabe-Sugano diagram, calculation of Dq, B, C, Nephelauxetic ratio.

Reaction mechanisms - substitution reactions in octahedral and square planar complexes, trans effect and its influence, water exchange, anation and base hydrolysis, stereochemistry, inner and outer sphere electron transfer mechanism.

Bioinorganic Chemistry: Transition metals in biology - their occurrence and function, active-site structure and function of metalloproteins and metalloenzymes with various transition metal ions and ligand systems; O2 binding properties of heme (haemoglobin and myoglobin) and non-heme proteins hemocynin & hemerythrin), their coordination geometry and electronic structure, co-operativity effect, Hill

coefficient and Bohr Effect; characterization of O2 bound species by Raman and infrared spectroscopic methods; representative synthetic models of heme and non-heme systems.

Electron transfer proteins - active site structure and functions of ferredoxin, rubridoxin and cytochromes, and their comparisons. Vitamin B12 and cytochrome P450 and their mechanisms of action.

Metals in medicine - therapeutic applications of cis-platin, transition metal radio-isotopes (example: Tc, Co and Cu etc.) and MRI (Mn and Fe) agents. Toxicity of metals - Cd, Hg and Cr toxic effects with specific examples.

Text Books:

1. M. Weller, T. Overton, J. Rourke and F. Armstrong, Inorganic Chemistry, 6th Edition, Oxford University Press, 2014. (South Asia Edition 2015)

2. J. E. Huheey, E. A. Keiter, R.L. Keiter and O. K. Mehdi, Inorganic Chemistry, Principles of Structure and Reactivity, 4th Edition, Pearson, 2006.

3. F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann, Advanced Inorganic Chemistry, 6th Edition, Wiley, 2007.

4. C. E. Housecroft and A. G. Sharpe, Inorganic Chemistry, 4th Edition, Pearson, 2012.

5. S. J. Lippard and J. M. Berg, Principles of Bioinorganic Chemistry, University Science Books, 1994.

6. W. Kaim and B. Schwederski and Axel Klein, Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life (An introduction and Guide), 2nd Edition, John Wiley & Sons, 2013.

CY5013: Conceptual Organic Chemistry

Class Hours	Expected Learning Hours by Students Outside the Class Hours	Total Credit
3	6	9

Course Objectives: To learn and apply various concepts such as stereochemistry and fundamental principles of stereoselectivity in organic chemistry.

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

Comprehend and **Predict** the role of temperature, solvents, and catalysts in organic reactions **Elucidate** reaction mechanisms using isotope effects

Identify and **differentiate** prochirality and chirality at centers, axis, planes and helices and determine the absolute configuration

Evaluate the stability of various conformers of acyclic and cyclic systems using steric, electronic and stereoelectronic effects and correlate them to reactivity. **Use** various models for determining stereoselectivity of various organic transformations

Course Contents:

Physical organic chemistry: Relationship between thermodynamic stability and rates of reactions – kinetic and thermodynamic control of product formation, Hammond's postulate, Curtin Hammett principle. Catalysis (acids, bases, and nucleophiles) and isotope effects, importance in the determination of organic reaction mechanisms, solvent effects, examples from SN2 and E2 reactions. Introduction to carbon acids, pKa of weak acids.
Stereochemistry: The concept of prochirality: topicity, prosteroisomerism, stereotopic ligands and faces and stereoheterotopic ligands, introduction to molecular symmetry and chirality, Center of chirality, molecules with C, N, S based chiral centers, axial, planar and helical chirality, stereochemistry and absolute configuration of allenes, biphenyls, binaphthyls, spiranes, exo-cyclic alkylidenecycloalkanes, ansa and cyclophanic compounds.

Conformational analysis: Introduction to conformational analysis, steric, electronic and stereoelectronic effects in governing the conformation of acyclic and cyclic (5 and 6 membered rings) systems, A-strains and anomeric effect, decalins, transannular interactions in medium size rings.

Conformation and reactivity: steric and electronic effects in syn-elimination, E2 elimination and neighboring group participation (Woodward, Prevost methods) of acyclic and cyclohexyl systems, esterification, substitution reaction and formation and opening of epoxide in cyclohexyl systems (Furst Plattner rule).

Stereoselectivity: Classification, terminology, principle of stereoselectivity, examples of diastereoselectivity using Cram, Cram-Chelate, Felkin-Ahn, anti-Felkin, Houk models, Cieplak and cation coordination models, and Zimmerman-Traxler transition

states, enantioselectivity. Desymmetrization and kinetic resolution, methods of determination of absolute configuration.

Text Books:

1. F. A. Carey and R. A. Sundberg, Advanced Organic Chemistry, Part A: Structure and Mechanisms, 5th Edition, Springer, New York, 2007.
2. T. H. Lowry and K. S. Richardson, Mechanism and theory in organic chemistry, Second edition, , Harper & Row, New York, 1981.
3. N. S. Isaacs, Physical Organic Chemistry, , ELBS, Longman, UK, 1987.
4. A. J. Kirby, Stereoelectronic effects, Oxford Chemistry Primers, 2011.
5. Steric and Stereoelectronic Effects in Organic Chemistry, V. K. Yadav, Springer, 2016.
6. D. Nasipuri,Stereochemistry of Organic Compounds. Principles and Applications, Second Edition, Wiley Eastern Limited, New Delhi, 1994. Ch.2-6 and 9-12.
7. D. G. Morris, Stereochemistry, RSC Tutorial Chemistry Text 1, 2001
8. E. L. Eliel and S. H. Wilen, Stereochemistry of Organic Compounds, John Wiley & Sons, New York, 1994.

CY5015: Classical and Statistical Thermodynamics

Class Hours	Expected Learning Hours by Students Outside the Class Hours	Total Credit
3	6	9

Course Objectives: The learners should be able to apply principles and laws of equilibrium thermodynamics to multicomponent systems. In addition, they should be able to use spectroscopic data to calculate thermodynamic properties of ideal gases, real gases, solids and metals using the principles and techniques of statistical thermodynamics.

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

Calculate change in thermodynamic properties, equilibrium constants, partial molar quantities, chemical potential. Identify factors affecting equilibrium constant.

Apply phase rule and, **draw** phase diagrams for one, and two component systems, **identify** the dependency of temperature and pressure on phase transitions, and **identify** first/second order phase transitions.

Solve problems based on Debye-Huckel limiting law. **Calculate** excess thermodynamic properties.

Calculate the absolute value of thermodynamic quantities (U, H, S, A, G) and equilibrium constant (K) from spectroscopic data.

Predict heat capacity (Cv, Cp) of an ideal gas of linear and non-linear molecules from the number of degrees of freedom, rotational and vibrational wave numbers.

Derive the temperature dependence of the second Virial coefficient (real gases) from interatomic potentials.

Explain T^3 dependence of heat capacity of solids at low temperatures (universal feature) using Debye and Einstein theory of heat capacity of solids.

Explain the concept of Fermi energy in metals and use it to calculate the chemical potential of conduction

Course Contents:

Classical Thermodynamics

Phase behavior of one and two component systems: Fundamental equations for open systems, Partial molar quantities and chemical potential, Chemical equilibrium, Phase behavior of one and two component systems, Ehrenfest classification of phase transitions.

Thermodynamics of mixtures: Thermodynamics of ideal and non-ideal solutions: Liquid-liquid solutions, liquid-solid solutions, multicomponent systems and excess thermodynamic properties, Activity of ideal, regular and ionic solutions.

Statistical Thermodynamics

Introduction: Concept of ensembles, partition functions and distributions, microcanonical, canonical and grand canonical ensembles, canonical and grand canonical partition functions, Boltzmann, Fermi-Dirac and Bose-Einstein distributions.

Ideal gases: Canonical partition function in terms of molecular partition function of non-interacting particles, Translational, rotational and vibrational partition functions. Absolute values of thermodynamic quantities (U,H,S,A,G) for ideal monoatomic and diatomic gases, heat capacity (Cv, Cp) of an ideal gas of linear and nonlinear molecules, chemical equilibrium.

Real gases: Canonical partition function for interacting particles, intermolecular potential (Lennard-Jones, Hard-sphere and Square-well) and virial coefficients. Temperature dependence of the second virial coefficient.

Solids: Thermodynamics of solids - Einstein and Debye models. T^3 dependence of heat capacity of solids at low temperatures (universal feature).

Metals: Fermi function, Fermi energy, free electron model and density of states, chemical potential of conduction electrons.

Text Books:

1. P. Atkins and J. Paula, Physical Chemistry, 10th Edition, Oxford University Press, Oxford 2014
2. D. A. McQuarrie and J. D. Simon, Molecular Thermodynamics, University Science Books, California 2004
3. R. S. Berry, S. A. Rice and J. Ross, Physical Chemistry, 2nd Edition, Oxford University Press, Oxford, 2007
4. D. A. McQuarrie, Statistical Mechanics, University Science Books, California 2005
5. B. Widom, Statistical Mechanics - A Concise Introduction for Chemists, Cambridge, University Press, 2002

CY5017: Principles of Quantum Mechanics

Credit Hours	Expected Learning Hours by Students Outside the Class Hours	Tutorial House	Total Credit
3	6	1	10

Course Objectives:

Revise and update the mathematical concepts of vectors and tensors to chemical systems by solving eigenvalue and eigenvector problems in matrices and first and second order differential equations that are used for solving the time independent Schrodinger equation.

Solve elementary model problems in quantum mechanics, particle in a potential-free box, particle on a ring, harmonic oscillator and particle in a Coulomb potential exactly and demonstrate the solutions for hydrogen atom and molecular rotations and vibrations.

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

Use mathematical techniques in linear algebra for eigenvalues and eigenvectors and first and second order differential equations not only in quantum chemistry but in other areas of physical and theoretical chemistry that will be offered during the whole programme.

Solve all the model problems in quantum mechanics for which exact analytical methods and solutions are available and will apply them to analyze the basis behind the postulatory method of quantum mechanics and which forms the foundations for advanced study of the subject.

Relate concepts that were originally introduced purely as modern atomic physics to molecular systems through harmonic oscillator, spin and rigid rotator.

Course Contents:

Mathematics

- Review of vectors and vector spaces, matrices and determinants, eigenvalues and eigenvectors, similarity transformations, ordinary differential equations- first and second order.

- Solution of differential equations by power series method: solutions of Hermite equation in detail. Orthogonality properties and recurrence relations. Introduction to the solutions of Legendre and Laguerre differential equations, Spherical Harmonics.

Quantum Mechanics

- Solution of the Schrodinger equation for exactly solvable problems for bound states such as particle-in-a- box, particle-in-a-ring, harmonic oscillator and rigid rotor.

- Postulates of quantum mechanics, wave functions and probabilities, operators, matrix representations, commutation relationships. Hermitian operators, Commutators and results of measurements in Quantum Mechanics. Eigenfunctions and eigenvalues of operators and superposition principle. States as probability distributions and expectation values. The expansion of arbitrary states in terms of complete set.

- Angular momentum, commutation relationships, basis functions and representation of angular momentum operators, Coupling (addition) of angular momenta

- Solution of the Schrodinger equation for the hydrogen atom, radial and angular probability distributions, atomic orbitals and electron spin, Pauli's exclusion principle and Aufbau principle.

- The time dependent Schrödinger equation. Co-ordinate and momentum space representation of operators and eigenstates; Role of Fourier transforms and simple examples; Unitary evolution and reversibility. Schrodinger and Heisenberg representations.

Text Books:

1. E. Kreyszig, Advanced Engineering Mathematics, 5th edition, Wiley Eastern, 1989.
2. G. Arfken and Hans J. Weber, Mathematical methods for physicists, Prism Indian Edition, 1995.
3. D. A. McQuarrie, Quantum Chemistry, University Science Books, 1983.
4. P. W. Atkins, Molecular Quantum Mechanics, 2nd edition, Oxford University Press, 1983.
5. I. N. Levine, Quantum Chemistry, 3rd edition, Allyn and Bacon, 1983.
6. D. J. Griffiths, Introduction to Quantum Mechanics, Pearson Education, 2005.
7. H. Kuhn, H.-D. Försterling, and D.H. Waldeck, Principles of Physical Chemistry, 2nd edition, Wiley, 2009.
8. J. P. Lowe, Quantum Chemistry, K. A. Peterson, 3rd edition, Academic Press, 2006.

CY5019: Organometallic Chemistry

Credit Hours	Expected Learning Hours by Students Outside the Class Hours	Total Credit
3	6	9

Course Objectives: The learners should be able to analyze the mechanism of selected catalytic organic reactions from the structure-bonding aspects and reactivity of simple organometallic compounds

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

Identify the structure and bonding aspects of simple organometallic compounds

Apply different electron counting rules to predict the shape/geometry of low and high nuclearity metal carbonyl clusters

Identify the different types of organometallic reactions and apply the above concepts to explain different catalytic reactions

Course Contents:

Organometallic chemistry of d-block elements: 18-electron rule, concept of hapticity; synthesis, structure and bonding of homo and heteroleptic metal-carbonyls, nitrosyls, alkyls, alkenes, allyl, alkynes, and arenes. Synthesis and reactivity of Fischer and Schrock carbenes.

Infrared spectra of metal carbonyls and olefins.
Neutral spectator ligands: phosphines and N-heterocyclic carbenes.

Metal clusters, Low and high nuclearity clusters, clusters having interstitial atoms, electron counting schemes:

polyhedral skeletal electron pair theory/Mingo's rule.

Structure and Isolobal analogies.

Metallocenes and bent-metallocenes.

Fluxionality and dynamics in organometallic chemistry

Reactions of organometallic complexes: Substitution, oxidative addition, reductive elimination, insertion and deinsertion.

Catalysis: Organometallic catalysts, Terminology in catalysis: Turnover, turnover number (TON), turnover frequency (TOF). Hydrogenation, Hydroformylation, Monsanto process, Wacker process, Ziegler-Natta polymerization, C-C coupling reactions, Olefin Metathesis and metathesis polymerization

Organometallic compounds of s-block elements: Organo-lithium, beryllium and magnesium compounds

Text Books:

1. M. Weller, T. Overton, J. Rourke and F. Armstrong, Inorganic Chemistry, 6th Edition, Oxford University Press, 2014. (South Asia Edition 2015)

2. J. E. Huheey, E. A. Keiter, R.L. Keiter and O. K. Mehdi, Inorganic Chemistry, Principles of Structure and Reactivity, 4th Edition, Pearson, 2006.

3. B. D. Gupta and A. J. Elias; Basic Organometallic Chemistry: Concepts, Synthesis, and Applications, 2nd Edition, Universities Press (India), 2013.

4. N. N. Greenwood and A. Earnshaw, Chemistry of the Elements, 2nd Edition, Elsevier, 1997.

5. P Powell, Principles of organometallic Chemistry, 2nd Edition, Springer, 2009.

CY5021: Introductory Computational Chemistry Laboratory

Class Hours	Total Credit
5	5

Course Objectives: The laboratory course is aimed at

Developing elementary programming skills in FORTRAN to enable them write short programs for performing scientific calculations.

Enabling to use graphical software for visualizing important mathematical functions and their properties through 2 D and 3 D graphs.

Introducing the basics of numerical mathematics using evaluation of functions, matrices and integrals.

Learning Outcomes

At the end of the course, the learners should be able to:

Write short simple programs in FORTRAN and be able to compile and execute them in a host of machines.

Use standard software tools such as MATLAB and Mathematica to **perform** algebraic and numerical calculations often required in elementary physical chemistry in the areas of quantum chemistry, spectroscopy, kinetics and thermodynamics

Use powerful 2D and 3D graphical packages of MATLAB and Mathematica to visualize almost any function of relevance in atomic orbitals, and probability densities in quantum chemistry and spectroscopy.

Course Contents:

The laboratory course is aimed at

Developing elementary programming skills in FORTRAN to enable them write short programs for performing scientific calculations

Enabling to use graphical software for visualizing important mathematical functions and their properties through 2 D and 3 D graphs

Introducing the basics of numerical mathematics using evaluation of functions, matrices and integrals.

Algebraic and numerical calculations using symbolic manipulation programs--Use of Mathematica for simple manipulations

Introduction FORTRAN 77 and FORTRAN 90 programming. Elementary exercises.

Matlab calculations and elementary programming exercises for Chemistry using algebraic programming and numerical exercises

Numerical matrix diagonalization of symmetric and hermitian matrices

Numerical techniques for integration: Gauss – Hermite quadrature method

Plotting atomic orbitals and calculating simple integrals involving hydrogen and several one-electron atoms. Introduction to elementary methods in numerical differentiation and integration

Introduction to Gaussian orbitals and wave functions and their visualizations. Orthogonalizing degenerate wave functions.

Introduction to Fourier transforms and the numerical fast Fourier transform method. Relations between time domain and frequency domain spectra.

Text Books:

1. William H. Press, Saul A. Teukolsky, William T. Vetterling and Brian P. Flannery, Numerical Recipes: The Art of Scientific Computing, 3rd Edition, Cambridge University Press, Cambridge, 2007.

2. Forman S. Acton, Numerical Methods that Work, Mathematical Association of USA, Washington D. C., 1990.

3. V. Rajaraman, Computer Programming using FORTRAN 77, Prentice-Hall of India, New Delhi, 2006.

4. V. Rajaraman, Computer Programming in FORTRAN 90 and 95, Prentice-Hall of India, New Delhi, 2006

5. MATLAB and Mathematica Programming manuals supplied by IIT Madras High Performance Computing Centre, IIT Madras.

CY5023: Organic Chemistry Laboratory

Class HoursTotal Credit 5
5

Course Objectives: The learners should be able to:

Apply principles of separation and isolation techniques in organic reactions.
Analyze NMR, IR and Mass spectra of organic compounds

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

Separate and **purify** products in organic reactions

Characterize organic compounds using spectroscopic and spectrometric techniques

Course Contents:

Separation of two-component mixtures of organic compounds. Synthesis and isolation of organic compounds with an emphasis on different techniques of reaction set-up (air-sensitive, moisture-sensitive etc.), separation/purification (extraction, Soxhlet extraction, recrystallization, distillation, column chromatography) and monitoring of reaction by TLC, Structure determination of the isolated pure compounds by NMR spectroscopy, IR Spectroscopy and Mass spectrometry.

Text Books:

In-House laboratory manual with the experimental procedures and relevant literature.

CY5012: Main Group Chemistry and Spectroscopic Characterization of Inorganic Compounds

Class Hours	Expected Learning Hours by Students Outside the Class Hours	Total Credit
3	6	9

Course Objectives: The learners should be able to apply, analyze and evaluate the structure and bonding aspects of inorganic and organometallic compounds derived from main group elements, using spectroscopic techniques.

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

Identify the basic principles related to structure and bonding of s & p block elements

Use various spectroscopic principles to characterize inorganic and organometallic compounds

Predict the synthesis and bonding properties of s and p block elements

Course Contents:

Structure and bonding in polyhedral boranes and carboranes, styx notation; Wade's rule; electron count in polyhedral boranes; synthesis of polyhedral boranes; isolobal analogy; boron halides; phosphine-boranes; borazine. Organyls of Al, Ga, In and Tl. Silanes, silicon halides, silicates, silanols; germanium, tin and lead organyls; phosphorous halides, acids and oxyacids, phosphazenes; sulphur halides, oxo acids of sulphur; structural features and reactivity of reactivity of S-N heterocycles; chemistry of halogens and group 18 elements.

Structural elucidation using the following spectroscopic techniques.

Symmetry and Point group analysis of simple inorganic compounds.
Electronic spectroscopy: electronic transitions in inorganic and organometallic compounds.

Infrared and Raman spectroscopy of simple inorganic molecules; predicting number of active modes of vibrations, analysis of representative spectra of metal complexes with various functional groups.

Applications of 1H and 13C NMR in inorganic and organometallic chemistry, fluxionality and dynamics; deriving activation and thermodynamic parameters; NMR spectral analyses of B, Al, Si, F and P containing compounds. Elementary aspects of Electron paramagnetic resonance (EPR) spectroscopy of inorganic compounds - g-values, hyperfine and super hyperfine coupling constants; selected applications in inorganic chemistry.

Mass spectrometry, basic principles, ionization techniques, isotope abundance, molecular ion; illustrative examples from supramolecules, inorganic/coordination and organometallic compounds.

Text Books:

1. M. Weller, T. Overton, J. Rourke and F. Armstrong, Inorganic Chemistry, 6th Edition, Oxford University Press, 2014. (South Asia Edition 2015)

2. J. E. Huheey, E. A. Keiter, R.L. Keiter and O. K. Mehdi, Inorganic Chemistry, Principles of Structure and Reactivity, 4th Edition, Pearson, 2006.

3. F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann, Advanced Inorganic Chemistry, 6th Edition, Wiley, 2007.

4. A. Abragam and B. Bleaney, Electron Paramagnetic Resonance of Transition Ions, Oxford University Press, 1970. (Reprint Edition 2013)

5. R. S. Drago, Physical Methods for Chemists, 2nd Edition,Saunders, 1992.

6. C. N. Banwell and E. M. McCash, Fundamentals of Molecular Spectroscopy, 4th Edition, McGraw-Hill, 1994.

7. H. Gunther, NMR Spectroscopy, Basic Principles, Concepts and Applications in Chemistry, 3rd Edition, Wiley VCH, 2013.

8. F. A. Cotton, Chemical Applications of Group Theory, Wiley, 3rd Edition, 1990. (Paperback 2008)

CY5014: Reactive Intermediates and Concerted Reactions

Class Hours	Expected Learning Hours by Students Outside the Class Hours	Total Credit
3	6	9

Course Objectives: To learn the involvement of reactive intermediates and understand their structure and reactivity through various organic reactions. To learn and understand the orbital interactions (Woodward Hoffmann rules) in concerted reactions. Learn to apply concerted and stepwise reactions in organic synthesis

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

Comprehend the structure-reactivity pattern of reactive intermediates involved in organic reactions

Comprehend the orbital interactions and orbital symmetry correlations of various pericyclic reactions

Write mechanism of organic reactions involving reactive intermediates and concerted processes

Apply these reactions in organic synthesis

Course Contents:

Carbanions: C-X bond (X = C, O, N) formations through the intermediacy of Carbanions: Chemistry of enolates and enamines, Kinetic and Thermodynamic enolates, Lithium and boron enolates in aldol and Michael reactions, Alkylation and acylation of enolates, Nucleophilic additions to carbonyls; Organolithium, Organomagnesium, Organozinc, Organocopper reagents (restricted to 1,4-addition) in synthesis, Name reactions under carbanion chemistry - Claisen, Dieckmann, Knoevenegal, Stobbe, Darzen, Acyloin condensations, Shapiro reaction, Julia olefination etc. Ylids: Chemistry of Phosphorous and Sulfur ylids - Wittig and related reactions, Peterson olefination etc.

Carbocation: Structure and stability of carbocations, Classical and non-classical carbocations, Neighbouring group participation and rearrangements including Wagner-Meerwein, Pinacol-pinacolone, semi-pinacol rearrangement, C-C bond formation involving carbocations, Oxymercuration, halolactonisation.

Carbenes and Nitrenes: Structure of carbenes, generation of carbenes, addition and insertion reactions, rearrangement reactions of carbenes such as Wolff rearrangement, generation and reactions of ylid by carbenoid decomposition, Structure of nitrene, generation and reactions of nitrene and related electron deficient nitrogen intermediates, Curtius, Hoffmann, Schmidt, Beckmann rearrangement reactions.

Radicals: Generation of radical intermediates and its (a) addition to alkenes, alkynes (inter & intramolecular) for C-C bond formation and Baldwin’s rules (b) fragmentation

and rearrangements. Name reactions involving radical intermediates such as Barton deoxygenation and decarboxylation, McMurry coupling etc.

Pericyclic Reactions: Classification, electrocyclic, sigmatropic, cycloaddition, chelotropic and ene reactions, Woodward Hoffmann rules, Frontier Orbital and Orbital symmetry correlation approaches, examples highlighting pericyclic reactions in organic synthesis such as Claisen, Cope, Diels-Alder and Ene reactions (with stereochemical aspects), dipolar cycloadditions and their utility in organic synthesis.

Text Books:

1. F. A. Carey and R. A. Sundberg, Advanced Organic Chemistry, Part B: Reactions and Synthesis, 5th edition, Springer, New York, 2007.

2. W. Carruthers and I. Coldham, Modern methods of Organic Synthesis, First South Asian Edition 2005, Cambridge University Press.

3. J. March and M. B. Smith, March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 6th Edition, Wiley, 2007.

4. I. Fleming, Frontier Orbitals and Organic Chemical Reactions, Wiley, London, 1976.

5. S. Sankararaman, Pericyclic Reactions- A text Book, Wiley VCH, 2005

CY5016: Kinetics and Reaction Dynamics

Class Hours	Expected Learning Hours by Students Outside the Class Hours	Total Credit
3	6	9

Course Objectives: The learners should be able to apply elementary laws of chemical kinetics and analyze reaction mechanisms and changes in transport properties of chemical reactions and collision processes

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

Calculate transport properties of gases, liquids and solids

Solve problems on rate/rate constants/efficiency for (i) complex reactions (ii) unimolecular and bimolecular reactions, and (iii) electronically excited state dynamics

Plot equations and functions representing kinetic behaviour of chemical systems in ground and electronically excited states

Course Contents:

Transport properties: Diffusion, Thermal conductivity, Viscosity, Effusion, Drift velocity, Nernst-Einstein equation, Stokes-Einstein equation Complex reactions-Chain reactions (free radical reaction, polymerization kinetics), Enzyme reaction, Inhibition kinetics

Temperature dependence of reaction rate: Linear and non-linear Arrhenius equation, Interpretation of Arrhenius parameters

Theories of reaction rates: Various theories of unimolecular reactions (Lindemann-Hinshelwood, RRK and RRKM theories), Potential energy surfaces for bimolecular reactions, Adiabatic and non-adiabatic curve crossing processes, Collision theory, Transition state theory, Activation/thermodynamic parameters, Erying equation

Kinetics in the excited state: Jablonski diagram, Kinetics of Unimolecular and bimolecular photophysical and photochemical processes, Quantum yield calculation, Excited state lifetime-quenching constant, Resonance energy transfer rates (RET), Rate and efficiency of RET, Dynamics of electron transfer, Solvent re-organization energy, Marcus theory of electron transfer, Free energy and rate relation, Rehm-Weller behaviour, Marcus Inverted Region

Text Books:

1. P. Atkins and J. Paula, Physical Chemistry, 10th edition, Oxford University Press, Oxford 2014
2. R. J. Silbey, R. A. Alberty, M. G. Bawendi, Physical Chemistry, 4th edition, Wiley-India, New Delhi 2005
3. R. S. Berry, S. A. Rice and J. Ross, Physical Chemistry, 2nd edition, Oxford University Press, Oxford 2007
4. K. J. Laidler, Chemical Kinetics, 3rd edition, Harper & Row, New York 1998
5. K. K. Rohatgi - Mukherjee, Fundamentals of Photochemistry, New Age International Pvt. Ltd.; 3rd edition, New Delhi 2014.
6. J. I. Steindeld, J. S. Francisco, W. L. Hase, Chemical Kinetics and Dynamics, 2nd edition, Prentice Hall International Inc., New York 1989

CY5018: Chemical Bonding and Group Theory

Class Hours	Expected Learning Hours by Students Outside the Class Hours	Total Credit
3	6	9

Course Objectives:

Recognize the most significant and elementary solutions of Schrodinger equation in molecular quantum mechanics through a study of time independent perturbation theory, valence bond and molecular orbital theories.

Apply the concept of linear combination of atomic orbitals to hybridization and directed bonding in polyatomic molecules.
Solve the real-world problem using advanced numerical programs through Gaussian orbitals.

Show that molecular symmetry operations form a group and can be characterized by fundamental representations of groups known as irreducible representations.

Apply the great orthogonality theorem to derive simple point groups and illustrate its use in the applications in crystal field theory, pericyclic reactions and molecular spectroscopy.

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

Apply time independent perturbation theory to complex problems of molecular energy levels in the presence of external electric and magnetic fields

Distinguish different types of hybridization based on geometries of the complex and to calculate for a one-electron and two electron system, all the necessary integrals due to coulombic forces.

Determine the symmetry operations of any small and medium-sized molecule and apply point group theory to the study of electrical, optical and magnetic properties and selection rules for absorption.

Course Contents:

- Time-independent perturbation theory, degenerate states, variational method, Hellmann-Feynman theorem Spectra and structure of helium atom, term symbols for atoms.
- Born-Oppenheimer approximation, hydrogen molecule ion, hydrogen molecule: valence bond and molecular orbital methods: Detailed calculations for energies and overlaps.
- Polyatomic molecules and hybridisation. Conjugated pi-systems and Huckel theory, frontier orbital theory, configuration interaction.

- Hartree-Fock method, self-consistent field method and derivation of Hartree-Fock, Roothaan Equations.
- Polyatomic basis sets, Gaussian, double-zeta and polarized basis sets, population analysis and dipole moments. The Thomas-Fermi model of the atom.

Group Theory in Chemistry

- The concept of groups, symmetry operations and symmetry elements in molecules, matrix representations of symmetry operations, point groups, irreducible representations and character tables.
- Great orthogonality theorem and its proof.
- Application of group theory to atomic orbitals in ligand fields, molecular orbitals, hybridization.
- Classification of normal vibrational modes, selection rules in vibrational and electronic spectroscopy. Woodward-Hoffmann rules.

Text Books:

1. D. A. McQuarrie, Quantum Chemistry, University Science Books, 1983.
2. P. W. Atkins, Molecular Quantum Mechanics, 2nd edition, Oxford University Press, 1983.
3. I. N. Levine, Quantum Chemistry, 3rd edition, Allyn and Bacon, 1983.
4. A. Szabo and N. S. Ostlund, Modern Quantum Chemistry, Dover, 1996.
5. R. McWeeney, Coulson's Valence, Oxford University Press, 1979.
6. F. A. Cotton, Chemical Applications of Group Theory, Wiley, 1996.
7. D. M. Bishop, Group theory and Chemistry, Dover, 1989.

CY5020: Analytical Chemistry: Principles, Practices and Applications

Class Hours	Expected Learning Hours by Students Outside the Class Hours	Total Credit
3	6	9

Course Objectives: The learners should be able to apply the conceptual understanding of the principles and implementation modes of several analytical instruments to chemical systems.

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

Solve problems based on various analytical concepts

Design experiments with improved sample preparation, new measurement procedures and tools

Quantify analytes with proper data handling and analysis

Design sensors

Course Contents:

Historical overview and the current status of analytical chemistry: an introduction.

Statistics for analytical experimentation: Probability, Regression analysis, Accuracy and propagation of errors, Data analysis and signal enhancement.

Advanced chromatographic techniques: Theory of separation methods: HPLC, GC, GC/MS, LC/MS, GPC, Supercritical fluid chromatography, Detectors in Chromatography, Applications of chromatography

Electroanalytical techniques: Applications to chemical & biological systems: Principles of Potentiometry, Electrogravimetry, Voltammetry, Stripping methods, Chronoamperometry, Quantitative applications of Potentiometry and Voltammetry: Electrochemical sensors, ISFETs, CHEMFETs.

Spectrometric and Spectroscopic methods: Acid-base equilibria, Methodology in spectrochemical analysis, Spectrophotometry and binding assays. Introduction to electromagnetic radiation, Optical components of a spectrometer, Sources (LASERS), Detectors. Atomic absorption and emission spectroscopy, Principles and applications of Fluorimetry, Dynamic light scattering. Preliminary analyses of a spectrum: Relative populations of species from intensity, Relate line widths to lifetime, Introduction to spectroscopy in time domain, Time-correlated single photon counting.

Physical methods of characterization: Surface Techniques: Principles and applications of electron spectroscopy for chemical analysis (ESCA) and Scanning Probe Microscopy.

Text Books:

1. D. A. Skoog, F. J. Holler and S. R. Crouch, Principles of Instrumental Analysis, 6th Edition, Brooks/Cole Cengage Learning, Belmont, CA, 2007

2. H. H. Willard, L. L. Merrln, Jr., J. A. Dean, and F. A. Senle, Jr., Instrumental Methods of Analysis: Wadsworth, 7th Edition, Belmont., 1989

3. F. Rousseac and A. Roessac, Chemical Analysis: Modern Instrumentation Methods and Analysis, 4th Edition, John Wiley & Sons, Ltd., 2000

4. J. Wang, Analytical Electrochemistry, 3rd Edition, Wiley – VCH, 2006

5. P.T. Kissinger and W. R. Heineman, Laboratory Techniques in Electroanalytical Chemistry, 2nd Edition, Marcel Dekker Inc., 1996

6. B. Voigtlaender, Scanning Probe Microscopy: Atomic Force Microscopy and Scanning Tunneling Microscopy:, Springer - Verlag, Berlin 2015

CY5022: Inorganic Chemistry Laboratory

Class Hours	Total Credit
5	5

Course Objectives: The learners should be able to apply the principles of qualitative and quantitative analytical techniques in inorganic chemistry for compound identification and characterization.

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

Plan and **Conduct** experiments for identifying and characterizing inorganic compounds

Course Contents:

Qualitative and quantitative estimations, synthesis, separation, purification, characterization and property measurements of inorganic compounds with an emphasis on different techniques of reaction set-up (air-sensitive, moisture-sensitive etc.). Exposure to various spectroscopic characterization techniques.

Text Books:

In-house laboratory manual and relevant literature

CY5024: Physical Chemistry Laboratory

Class HoursTotal Credit 55

Course Objectives: The learners should be able to validate the conceptual understanding acquired from the theory classes

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

Explain the principle behind the experiments performed in the laboratory

Plan and **Perform** experiments and **Interpret** experimental results

Course Contents:

Experiments on thermodynamics, kinetics, catalysis, electrochemistry, photochemistry, spectroscopy, and macromolecules.

Text Books:

1. B. Viswanathan, and P. S. Raghavan, Practical Physical Chemistry, Viva Books, 2010

2. A. M. Halpern, and G. C. McBane, Experimental Physical Chemistry: A Laboratory Text Book, 3rd Edition, W. H. Freeman, 2006

CY6011: Solid State Chemistry

Class Hours	Expected Learning Hours by Students Outside the Class Hours	Total Credit
3	6	9

Course Objectives: To identify and apply the concepts involved in the syntheses, structure and physical properties of crystalline inorganic solids

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

Arrive at the chemical compositions based on unit cell contents and fractional coordinates.

Index cubic powder XRD pattern, determine unit cell parameter and lattice type

Index non-cubic powder XRD patterns based on unit cell parameters provided **Calculate** densities from powder XRD data **Identify** and **apply** a suitable strategies for synthesizing inorganic crystalline solids in polycrystalline and single crystal forms **Correlate** and **Predict** structure-composition-properties (magnetic, electrical and optical) in inorganic crystalline solids

Course Contents:

Crystal Structure: Crystalline and amorphous solids; One and two dimensional lattices, crystal systems, Bravais lattices, point groups: α-Po, fcc, bcc and hcp metals and their packing efficiency, ionic radii ratios; structure types of ionic solids: CsCl, NaCl, ZnS, Na2O, CaF2, CdCl2, NiAs, ZnO, CdI2, Cs2O, PbO, TiO2, ReO3, perovskite ABO3, YBa2Cu3O7, K2NiF4, Ag2HgI4, spinel and olivine. Polyhedral structure description of solid state compounds. Frenkel and Schotky defects, colour centers, Crystallographic shear (CS) in WO3-x

Powder x-ray diffraction, indexing the powder XRD patterns, Systematic absences, Structure factor, determination of lattice type, unit cell parameter and density for α-Po, fcc, bcc and hcp metals, NaCl, ZnS, diamond, CuZn, CuAu, AuCu3 and other simple compounds. Neutron diffraction.

Preparative methods: Solid state reaction, chemical precursor method, co-precipitation, sol-gel, metathesis, self-propagating high temperature synthesis, ion-exchange reactions, intercalation / deintercalation reactions; hydrothermal and template synthesis; High pressure synthesis.

Methods of Single Crystal Growth: Solution growth; Melt Growth-Bridgeman, Czochralski, Kyropoulus, Verneuil; Chemical Vapour Transport; Fused Salt Electrolysis; Hydrothermal method; Flux Growth.

Electrical properties: Band theory of solids -metals and their properties; semiconductors - extrinsic and intrinsic, Hall effect; thermoelectric effects (Thomson, Peltier and Seebeck); insulators - dielectric, ferroelectric, pyroelectric and piezoelectric properties, multiferroics.

Superconductivity: Basics, discovery and high Tc materials.

Magnetic properties: Dia, para, ferro, ferri, and antiferro magnetic types; soft and hard magnetic materials; select magnetic materials such as spinels, garnets and perovskites, hexaferrites and lanthanide-transition metal compounds; magnetoresistance.

Thermal analysis: TGA, DTA, DSC

Text Books:

1. A. R. West, Solid State Chemistry and its Applications, John Wiley & Sons, 1984. (Reprint Edition)
2. L. E. Smart and E. A. Moore, Solid State Chemistry - An Introduction, 4th Edition, CRC Press, 2012.
3. H. V. Keer, Principles of the Solid State, 2nd Edition, New Age International, 2017.
4. M. Weller, T. Overton, J. Rourke and F. Armstrong, Inorganic Chemistry, 6th Edition, Oxford University Press, 2014. (South Asia Edition 2015)

CY6013: Spectroscopy-Applications in Organic Chemistry

Class Hours	Expected Learning Hours by Students Outside the Class Hours	Total Credit
3	6	9

Course Objectives: To learn basic principles of NMR, IR, UV-Vis spectroscopy and mass spectrometry and to use these spectroscopic methods for organic structure elucidation.

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

Apply NMR, IR, MS, UV-Vis spectroscopic techniques in solving structure of organic molecules and in determination of their stereochemistry.

Interpret the above spectroscopic data of unknown compounds.

Use these spectroscopic techniques in their research.

Course Contents:

NMR Spectroscopy: NMR phenomenon, spin ½ nuclei, (1H, 13C, 31P and 19F), 1H NMR, Zeeman splitting, effect of magnetic field strength on sensitivity and resolution, chemical shift δ, inductive and anisotropic effects on δ, chemical structure correlations of δ, chemical and magnetic equivalence of spins, spin-spin coupling, structural correlation to coupling constant J, first order patterns. Second order effects, examples of AB, AX, AA'BB' and ABX systems, simplification of second order spectrum, application of NMR data for stereochemical assignments, selective decoupling, use of chemical shift reagents for stereochemical assignments. 13C NMR, introduction to FT technique, relaxation of nuclear spins, NOE effects, 1H and 13C chemical shifts to structure correlations. Study of dynamic processes by VT NMR, restricted rotation (DMF, DMA, biphenyls, annulenes), cyclohexane ring inversion, degenerate rearrangements (bullvalene and related systems).

Application of DEPT technique to the analysis of CH multiplicities in 13C NMR spectroscopy.

Correlation spectroscopy: Illustration of practical applications of 1H-1H COSY, 1H-13C COSY, NOE difference spectroscopy (Stereochemistry determination), HMQC and HSQC techniques.

Electronic spectroscopy, basic principle, electronic transitions in organic, and molecules and application to structure elucidation. Optical rotatory dispersion and circular dichroism (ORD and CD) spectroscopy, underlying principle, Plane curves, Cotton effects, octant rule, axial halo-keto rule, applications to assignment of configuration of chiral molecules. Infrared spectroscopy: organic functional group identification through IR spectroscopy.

Mass spectrometry:, basic principles, ionization techniques, isotope abundance, molecular ion, fragmentation processes of organic molecules, deduction of structure through mass spectral fragmentation, high resolution MS, soft ionization methods, ESI-MS and MALDI-MS, basic principle of ionization and ion analysis, illustrative examples from simple organic molecules to macromolecules and supramolecules. Structure elucidation problems using the above spectroscopic techniques.

Text Books:

1. H. Gunther, NMR Spectroscopy, 2nd ed.; John Wiley and Sons, 1995.
2. D. L. Pavia, G. M. Lampman, G. S. Kriz, J. R. Vyvyan, Spectroscopy, Cengage Learning, New Delhi, 2007.
3. W. Kemp, Organic Spectroscopy, 2nd edition, ELBS-Macmillan, 1987.
4. T. D. W. Claridge, High Resolution NMR Techniques on Organic Chemistry, Pergamon, New York, 1999.
5. R. S. Macomber, A Complete Introduction to Modern NMR Spectroscopy, R. S. Macomber, Wiley, 1997.
6. For CD and ORD: D. Nasipuri, Stereochemistry of Organic Compounds, Principles and Applications, New Age International, New Delhi, 2011, chapter 15.

CY6015: Electrochemistry: Fundamentals and Applications

Class Hours	Expected Learning Hours by Students Outside the Class Hours	Total Credit
3	6	9

Course Objectives: The learners should be able to apply theories in electrochemistry to analyze electrode kinetics.

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

Write equations representing electrochemical cell, **explain** various overpotential involved during the operation of the cell.

Calculate electrochemical cell parameters, electrochemical active surface area, current and overpotential under given condition, amount of corrosion and its rate

Plot potential vs current, surface coverage vs. potential, potential vs. pH, concentration profile vs. distance from the electrode

Course Contents:

Ionics: Electrochemistry of solutions, Ion-solvent interactions, ion-ion interactions, ionic migration and diffusion. Phenomenological description of transport processes. Thermodynamics of galvanic cells: Equilibrium electrode potentials, IUPAC convention for electrode potentials, Thermodynamics of electrochemical cells and applications.

Electrical Double layer: Theories of Double-Layer structure, diffuse-double-layer theory of Gouy and Chapman, the Stern Model, Adsorption of ions and neutral compounds, Electrocaplillary and differential capacitance measurements; Influence of double layer on charge transfer processes.

Reference electrodes: polarizable and non-polarizable systems. Types of reference and working electrodes

Electrode kinetics: Current-potential relationship (derivation of Butler-Volmer and Tafel equations). Adsorption isotherms for intermediates formed by charge transfer (Langmuir adsorption and its limitations, relating bulk concentration to surface coverage), Types of overpotentials: origin and minimization; mechanism of electro-organic reactions; hydrogen evolution and oxygen reduction reactions. transition state theory and Gibbs free energy of activation, bulk electrolysis; Quadratic activation –driving force relation –Marcus theory ; outer and inner sphere reactions. Underpotential deposition of metals and applications in catalysis.

Corrosion: Different types of corrosion; influence of environment; Evans diagram, Pourbaix diagram; corrosion rate measurements; Stern Geary equation; mixed potential theory and prevention of corrosion.

Text Books:

1. E. Gileadi, Physical Electrochemistry, Fundamental, Techniques and Applications, Wiley-VCH, 2011
2. A. J. Bard and L. R Faulkner Electrochemical Methods: Fundamentals and Applications, 2nd Edition, Wiley, 2001
3. P. H. Rieger, Electrochemistry, 2nd Edition, Springer 1994
4. J. Newman and K. E. Thomas-Alyea, Electrochemical Systems, 3rd Edition, Wiley Interscience, 2004

CY6017: Optical and Magnetic Resonance Spectroscopy

Class Hours	Expected Learning Hours by Students Outside the Class Hours	Total Credit
3	6	9

Course Objectives:

Recognize the fundamental principles of optical and magnetic resonance through both theory and examples drawn from molecular literature, Derive the Fermi's Golden Rule and simple relations between experimentally observable spectroscopic quantities and molecule dependent parameters by introducing time dependent quantum mechanics and show that spectroscopy connects matter with molecules through interaction of electromagnetic radiation.

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

Connect the spectroscopic line positions (frequencies), line intensities and line widths with a single approximate formula given by Enrico Fermi.

Apply principles of microwave, infrared and electronic spectroscopies to identify the fingerprint region of small molecules in gas and solution phases.

Apply the concept of chemical shift and spin-spin coupling in both NMR and EPR spectroscopy to identify high resolution spectra of small organic molecules.

Apply the concepts learnt in the course to the general study of spectra of a large class of inorganic and organic compounds given in other courses in M.Sc.

Course Contents:

Introduction

Interaction of radiation with matter, Einstein coefficients, time dependent perturbation theory, transition probability, transition dipole moments and selection rules, factors that control spectral linewidth and lineshape. Beer-Lambert law and absorbance.

Molecular Spectroscopy

The rigid diatomic rotor, energy eigenvalues and eigenstates, selection rules, intensity of rotational transitions, the role of rotational level degeneracy, the role of nuclear spin in determining allowed rotational energy levels. Classification of polyatomic rotors and the non-rigid rotor.

Vibrational spectroscopy, harmonic and anharmonic oscillators, Morse potential, mechanical and electrical anharmonicity, selection rules. The determination of anharmoncity constant and equilibrium vibrational frequency from fundamental and overtones. Normal modes of vibration, G and F matrices, internal and symmetry coordinates.
Electronic transitions, Franck-Condon principle. Vertical transitions. Selection rules, parity, symmetry and spin selection rules. Polarization of transitions. Fluorescence and phosphorescence.

Raman spectroscopy, polarizability and selection rules for rotation and vibrational Raman spectra.

Magnetic Resonance

Expression for Hamiltonian/Energy - Zeeman interaction, torque exerted by a magnetic field on spins, equation, its solution and the physical picture of precession. Thermal equilibrium, Curie susceptibility. Expressions for MR spectral sensitivity. Approach to equilibrium, Bloch equations, the rotating frame, Steady state (continuous wave) and Transient (pulsed) experiments, solutions of classical master equation. Absorption and dispersion in cw and pulse experiments, the complex Fourier transform. Field modulation in cw MR and derivative EPR lineshapes. The spin Hamiltonian, isotropic and anisotropic interactions.

The EPR Hamiltonian. Theory of g-factors in EPR, transition metal complexes, rare earth complexes. Theory of hyperfine interactions in π−type free radicals, McConnell relation. The NMR Hamiltonian, shifts and couplings. The Solomon equations and cross-relaxation, the Overhauser effect, steady state NOE, sensitivity enhancement, transient NOE, interatomic distance information.

The spin echo. Vector picture and algebraic expressions for effect on spin evolution under field inhomogeneities, chemical shifts and homonuclear/heteronuclear couplings, the basis of heteronuclear decoupling.

Polarization transfer. Selective Population Inversion, INEPT and RINEPT, sensitivity enhancement and spectral editing.

Text Books:

1. P. W. Atkins, Molecular Quantum Mechanics, 2nd edition, Oxford University Press, 1983.
2. P. F. Bernath, Spectra of Atoms and Molecules, 2nd Edition, Oxford University Press, 2005.
3. E. B. Wilson, Jr., J. C. Decius and P. C. Cross, Molecular Vibrations: The Theory of Infrared and Raman Spectra, Dover Publications, 1980.
4. W. Demtroder, Molecular Physics, Wiley-VCH, 2005.
5. J. A. Weil and J. R. Bolton, (Eds), Electron Paramagnetic Resonance: Elementary Theory and Practical Applications, Second Edition, Wiley Interscience, John Wiley & Sons, Inc., 2007.
6. A. E. Derome, Modern NMR Techniques for Chemistry Research, Pregamon, 1987.
7. C. P. Slichter, Principles of Magnetic Resonance, Third Edition, Springer-Verlag, 1990.
8. T. C. Farrar and E. D. Becker, Pulse and Fourier Transform NMR, Academic Press, New York, 1971.

CY6019: Modern Synthetic Methodology in Organic Chemistry
(Department Elective-I)

Class Hours	Expected Learning Hours by Students Outside the Class Hours	Total Credit
3	6	9

Course Objectives: To learn various organic reactions and reagents used in them as tools applied in the art of organic synthesis. To learn retrosynthetic approach towards organic synthesis.

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

Use various reagents and organic reactions in a logical manner in organic synthesis.

Use retrosynthetic method for the logical dissection of complex organic molecules and devise synthetic methods

Course Contents:

Oxidation: Metal based and non-metal based oxidations of alcohols (chromium, manganese, silver, ruthenium, DMSO, and hypervalent iodine). (b) Peracids oxidation of alkenes and carbonyls. (c) Alkenes to diols (manganese, osmium based), alkenes to carbonyls with bond cleavage (manganese, ruthenium, and lead based, ozonolysis), and alkenes to alcohols/carbonyls without bond cleavage (hydroboration-oxidation, Wacker oxidation, and selenium based allylic oxidation). (d) Asymmetric epoxidations (Sharpless, Jacobsen, and Shi epoxidations) and Sharpless asymmetric dihydroxylation.

Reduction: (a) Catalytic homogeneous and heterogeneous hydrogenation, Wilkinson catalyst. (b) Metal based reductions using Li/Na in liquid ammonia, sodium, magnesium, zinc, titanium, and samarium. (c) Hydride transfer reagents: $NaBH_4$, L-selectride, K-selectride, Luche reduction, $LiAlH_4$, DIBAL-H, Red-Al, Trialkylsilanes, and Trialkylstannane. (d) Enantioselective reductions (Chiral Boranes, Corey-Bakshi-Shibata) and Noyori asymmetric hydrogenation.

Modern Synthetic Methods: (a) Baylis-Hillman reaction, Henry reaction, Kulinkovich reaction, Ritter reaction, Sakurai reaction, Brook rearrangement, Tebbe olefination. (b) Metal mediated C-C and C-X coupling reactions: Heck, Stille, Suzuki, Negishi and Sonogashira, Nozaki-Hiyama, Buchwald-Hartwig, Ullmann coupling reactions, directed ortho metalation. (c) Stereoselective synthesis of tri- and tetra-substituted olefins, Synthetic applications of Claisen rearrangement, ene reaction (metallo-ene, Conia ene).

Construction of Ring Systems: (a) Different approaches towards the synthesis of three, four, five, and six-membered rings. (b) Pauson-Khand reaction, Bergman cyclization; Nazarov cyclization, cation-olefin cyclization and radical-olefin cyclization, inter-conversion of ring systems (contraction and expansion). (c) Construction of macrocyclic rings and ring closing metathesis.

Retrosynthetic Analysis: Basic principles and terminology of retrosynthesis, synthesis of aromatic compounds, one group and two group C-X disconnections, one group C-C and two group C-C disconnections, amine and alkene synthesis, important strategies of retrosynthesis, functional group transposition, important functional group interconversions Protecting groups: Protection and deprotection of hydroxy, carboxyl, carbonyl, carboxy amino groups and carbon-carbon multiple bonds; chemo- and regioselective protection and deprotection; illustration of protection and deprotection in synthesis.

Text Books:

1. W. Carruthers, Modern Methods of Organic Synthesis, Cambridge University Press, 1996.
2. L. Kuerti and B. Czako, Strategic Applications of named Reactions in Organic Synthesis, Elsevier Academic Press, 2005.
3. J. Clayden, N. Greeves, S. Warren and P. Wothers, Organic Chemistry, Oxford University Press, 2001.
4. F. A. Cary and R. I. Sundberg, Advanced Organic Chemistry, Part A and B, 5th Edition, Springer, 2009.
5. M. B. Smith, Organic Synthesis, 2nd Edition, 2005
6. S. Warren, Organic Synthesis, The disconnection Approach, John Wiley & Sons, 2004.
7. J. Tsuji, Palladium Reagents and Catalysts, New Perspectives for the 21st Century, John Wiley & Sons, 2003.
8. I. Ojima, Catalytic Asymmetric Synthesis, 2nd edition, Wiley−VCH, New York, 2000.
9. R. Noyori, Asymmetric Catalysis in Organic Synthesis, John Wiley & Sons, 1994.

CY6023: New Methods and Strategies in Organic Synthesis
(Department Elective-II)

Class Hours	Expected Learning Hours by Students Outside the Class Hours	Total Credit
3	6	9

Course Objectives: To learn various organic reactions and reagents used in them as tools applied in the art of organic synthesis. To learn retrosynthetic approach towards organic synthesis.

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

Use various reagents and organic reactions in organic synthesis

Use retrosynthetic method for the logical dissection of complex organic molecules and devise synthetic methods

Course Contents:

Chemo-, regio- and stereoselective functional groups interconversions; oxidation and reduction processes and their synthetic utility; metal-free oxidation (boron-, peroxide-, sulfur-, iodine-based) and metal-based (Ru-, Cr-, Mn-, Os-, Pd-) reagents; transfer hydrogenation; enantioselective oxidation and reduction processes.

Strategic carbon-carbon and carbon-heteroatom bonds formation; carbon-carbon multiple bonds construction processes and corresponding named reactions; functional group transposition; conjunctive reagents; construction of cyclic frameworks; fused and spirocyclic systems.

Domino/Cascade reactions: principles and advantages; rationalization with examples of radical, anionic, cationic, and pericyclic domino/cascade processes.

Metal catalyzed/promoted and metal-free cross-coupling and annulation reactions: Pd-, Cu-, Ni-, Fe-, Co-, Ru-catalyzed reactions; concept of C–H bond activation/functionalization.

Strategic bond disconnection, disconnection approach towards small molecules and natural products; protection and deprotection of oxygen and nitrogen containing common functional groups; protecting group free organic synthesis.

Text Books:

1. W. Carruthers, Modern Methods of Organic Synthesis, Cambridge University Press, 1996
2. L. Kuerti and B. Czako, Strategic Applications of named Reactions in Organic Synthesis, Elsevier Academic Press, 2005
3. F. A. Cary and R. I. Sundberg, Advanced Organic Chemistry, Part A and B, 5th Edition, Springer, 2009
4. J. Clayden, N. Greeves, and S. Warren, Organic Chemistry, Oxford University Press, 2nd Edition, 2012
5. L. F. Tietze, G. Brasche, and K. Gericke, Domino Reactions in Organic Synthesis, Wiley, 2006
6. Roderick Bates, Organic Synthesis using Transition Metals, 2nd Edition, Wiley, 2012
7. George S. Zweifel and Michael H. Nantz, Modern Organic Synthesis: An Introduction, W. H. Freeman Publisher, 2007.
8. S. Warren, Organic Synthesis, The disconnection Approach, John Wiley & Sons, 2004.

Choice Based Learning: Project

M. Sc. Project provides adequate training in conducting cutting edge research in the areas of modern chemistry. Those students who wish to take up research as a career may want to utilize this option. All students are encouraged to register for this course.

The projects are offered by the faculty of Department of Chemistry, individually or through collaboration with faculty of any other department in the Institute. In any case, the main guide will always be a faculty from Department of Chemistry. Students are free to interact with all faculty members of the department at the end of the second semester to decide the project in which they would like to work.

The total credit of the course is 27 and it is spread through the third and fourth semesters (9 and 18, respectively). Please refer the credit structure given in page 4.

Students engaged in research project from the beginning of 3rd semester will be subjected to Mid-Term evaluation at the end of 3rd semester.

(a) Students with satisfactory performance will continue with their research project in 4th semester, along with 3 electives of their choice, as their course work.

(b) Students with unsatisfactory performance and recommended for discontinuation of the research project, will have to take 6 elective courses during the 4th semester

(c) For any reason, if a student wishes NOT to take the project, she/he can do so by registering to a total of 6 electives in the fourth semester.

Choice Based Learning: Electives

Department of Chemistry offers a number of electives to promote choice based learning through the Program.

During the third semester, students elect one of the following two courses:

CY6019: Modern Synthetic Methodology in Organic Chemistry (Department Elective-I)

Or

CY6023: New Methods and Strategies in Organic Synthesis (Department Elective-II)

As mentioned in page number 42, students who take up the project course will have to register for three more electives in the fourth semester. Chemistry office will provide the list of elective courses offered every semester.

Students with un-satisfactory performance in the project will have to dis-continue the project at the end of 3rd semester and they should take six elective courses in the 4th semester.

Students who do not take up the project have to register for six elective courses in the fourth semester.

ELECTIVE COURSES

CY 6101 - Magnetic Resonance Imaging

Introduction to Magnetic Resonance - Principles of Spatial encoding in Magnetic Resonance - application of magnetic field gradients - Larmor frequency as a function of position - frequency encoding - the generation of profiles in NMR and ESR experiments run in the presence of gradients

Combination of frequency encoding with phase encoding for 2D imaging; ‗field of view' in phase and frequency directions; the basic Fourier imaging experiment (‗spin warp imaging') - gradient echoes; spin echo imaging; chemical shift selective imaging

Reciprocal space (*k* space) description of imaging experiments - parallel, radial and single pass raster techniques

Slice selection for 2D imaging - shaped pulses and slice profiles; slice thickness as a function of selective pulse bandwidth and slice gradient; gradient trimming for magnetization refocusing; multiple slice selection

3D Fourier imaging with two phase encode gradients; Echo Planar

Imaging Metabolite imaging; Diffusion weighted imaging; flow imaging

Materials and *in vivo* applications

Multiple Quantum (mq) imaging - point scan in *k* space with phase encoding alone; combination of mq phase encode with sq frequency encode for line scans in *k* space; applications to polymers, solution state and lyotropics

Spectral-Spatial imaging - chemical shift imaging (csi); mq-csi

NMR Imaging of solids - stray field imaging (STRAFI); projection reconstruction imaging

CW ESR imaging

Volume selective spectroscopy

Text Books:

1. P. Mansfield and P. Morris, ―NMR Imaging in BioMedicine‖, Academic Press, NY (1982)
2. P.T. Callaghan, Principles of NMR Microscopy, Oxford (1991/1994)
3. R. Kimmich, NMR Tomography, Diffusometry, Relaxometry, Springer (1997)
4. B. Blümich, NMR imaging of materials, Oxford (2000)

CY 6102 - Advanced Bioinorganic Chemistry

Essential and trace metal ions in biology and their distribution, thermodynamic and kinetic factors for the presence of selected metal ions; bioligands- amino acids, proteins, nucleic acids, nucleotides and their potential metal- binding sites; special ligands - porphyrins, chlorin and corrin.

Enzymes- Nomenclature and classification, chemical kinetics, the free energy of activation and the effects of catalysts kinetics of enzyme catalyzed reactions- Michaelis-Menten constant- effect of pH, temperature on enzyme reactions, factors contributing to the catalytic efficiency of enzymes.

O_2 binding and activation by heme, non-heme and copper proteins – MMO & RNR, tyrosinase; DβM, PHM, Cytochrome c oxidase.

Iron transport and storage proteins in bacterial and mammalian systems – siderophores, transferrin, ferritin.

Electron transport proteins – redox properties, organic- redox protein cofactors – FAD, NAD, FMN, ubiquinone; blue copper proteins, cytochromes, iron- sulfur proteins – rubredoxin, ferridoxins, HIPIP; electron transport chain (ETC) in respiration, nitrogen-fixation and photosynthesis.

Nitrogen-cycle enzymes: Mo in N, and S-metabolism by Mo-pterin cofactors and Mo-Fe-cofactors. NOx reductases, sulfite oxidase, xanthine oxidase, nitrogenase, P and M- clusters in nitrogenase, transition-metal-dinitrogen complexes and insights into N_2 binding, reduction to ammonia.

Mn in photosynthesis and O_2 evolution: Photosystem I and II – chlorophyll, oxygen evolving complex (OEC), 4Mn-cluster and O_2 evolution.

Non-redox enzymes with Mg, Zn, Ni: urease, peptidases and phosphatases and their structure and function. Carbonic anhydrase and carboxy peptidase.

Applied bioinorganic chem–metals in medicine, anti-cancer agents–cisplatin, radiopharmaceuticals (Tc), diagnostic (Gd in MRI) and therapeutic agents. Toxicity of Hg, Cd, Pb and As and chelation therapy.

Text Books:

1. Principle of Bioinorganic chemistry – Lippard and Berg, Univ. Science Books, 1994.
2. Biocoordination chemistry – Fenton, Oxford chemistry primer, 1995.
3. Bioinorganic chemistry: Inorganic perspective in the chemistry of Life, Kaim and Schwederski, 1994.
4. Inorganic chemistry – Shriver, Atkins, and Langford, 1994.
5. Bioinorganic Chemistry – Bertini, Gray, Lippard and Valentine Viva books Pvt. Ltd. 1998.

CY 6103 - Chemistry of Crystalline Inorganic Solid State Materials

Synthesis, structure, properties, structure-property correlations and potential applications of crystalline inorganic solid state materials.

Superconductors – (Ba,K)BiO_3, Cuprates, LnFeAsO, MgB_2, CaC_6

CMR materials – $La_{1-x}Sr_xMnO_3$

Ferroic compounds – $BaTiO_3$, $PbTiO_3$, $Bi_4Ti_3O_{12}$, $SrRuO_3$

Photoluminescent materials – Lanthanide compounds Porous materials – zeolites, AlPO, MeAlPO, SAPO.

Organic-inorganic hybrid materials – Ruddlesden-Popper $(RNH_3)_2A_{n-1}MX_{3n+1}$ metal halides, MOF compounds

Ionic Conductors – NASICON, AgI, $NaAl_{11}O_{17}$

Thermoelectric materials – Na_xCoO_2, $AgSbTe_2$, $CoSb_3$, $Y_{14}MnSb_{11}$

Compounds for intercalation and redox reactions – $LiCoO_2$, $LiVS_2$, NASICON, Chevrel phases

Other relevant examples from recent literature

Text Books:

1. Rao, C.N.R.; Gopalakrishnan, J. *New directions in Solid State Chemistry*; Cambridge University Press: Cambridge, 1997 (ISBN 0-521-49907-0).
2. Cheetham, A.K. *Solid state chemistry: compounds*; Oxford University Press: Oxford, 1992 (ISBN: 0198551665, 9780198551669).
3. Lalena, J.N.; Cleary, D.A. *Principles of Inorganic Materials Design* ; Wiley: New York, 2010 (ISBN: 978-0-470-40403-4).
4. Maier, J. *Physical Chemistry of Ionic Materials: Ions and Electrons in Solids*; Wiley: New York, 2004 (ISBN: 978-0-470-87076-1).
5. *Solid-state Chemistry of Inorganic Materials VI (SYMPOSIUM QQ AT THE 2006 MRS FALL MEETING)*; Curran Associates, Inc., 2007 (ISBN: 1558997962).

CY 6104 - Molecular Clusters

Introduction to molecular clusters

Main-group clusters: Geometric and electronic structure, three-, four- and higher connect clusters, the *closo-, nido-, arachno*-borane structural paradigm, Wade-Mingos and Jemmis electron counting rules, clusters with nuclearity 4-12 and beyond 12. Structure, synthesis and reactivity.

Transition-metal clusters: Low nuclearity metal-carbonyl clusters and 14n+2 rule, high nuclearity metal-carbonyl clusters with internal atoms. Structure, synthesis and reactivity. Capping rules, isolobal relationships between main-group and transition metal fragments, metal-ligand complexes vs heteronuclear cluster.

Main-group-Transition-metal clusters: Isolobal analogs of p-block and d-block clusters, limitations and exceptions.

Clusters having interstitial main group elements, cubane clusters and naked or Zintl clusters.

Molecular clusters in catalysis, clusters to materials, boron-carbides and metal-borides.

Illustrative examples from recent literature.

Text Books:

1. D. M. P. Mingos and D. J. Wales; Introduction to Cluster Chemistry, Prentice Hall, 1990.
2. N. N. Greenwood and E. A. Earnshaw; Chemistry of elements, Second Edition, Butterworth- Heinemann, 1997.
3. T. P. Fehlner, J. F. Halet and J-Y. Saillard; Molecular Clusters: A Bridge to solid-state Chemistry, Cambridge University press, 2007.
4. B. D. Gupta and A. J. Elias; Basic Organometallic Chemistry: Concepts, Synthesis, and Applications, Universities Press (India), 2010.
5. D. M. P. Mingos, Essential Trends in Inorganic Chemistry, Oxford, University Press, 1998.
6. C. E. Housecroft, Metal-Metal Bonded Carbonyl Dimers and Clusters, Oxford Chemistry Primers (44), Oxford, University Press, 1996.

CY 6105 - Supramolecular Chemistry

Definition of supramolecular chemistry. Nature of binding interactions in supramolecular structures: ion-ion, ion-dipole, dipole-dipole, H-bonding, cation-p, anion-p, p-p, and van der Waals interactions.

Synthesis and structure of crown ethers, lariat ethers, podands, cryptands, spherands, calixarenes, cyclodextrins, cyclophanes, cryptophanes, carcerands and hemicarcerands., Host-Guest interactions, pre-organization and complimentarity, lock and key analogy. Binding of cationic, anionic, ion pair and neutral guest molecules.

Crystal engineering: role of H-bonding and other weak interactions.

Self-assembly molecules: design, synthesis and properties of the molecules, self assembling by H-bonding, metal-ligand interactions and other weak interactions, metallomacrocycles, catenanes, rotaxanes, helicates and knots.

Molecular devices: molecular electronic devices, molecular wires, molecular rectifiers, molecular switches, molecular logic.

Relevance of supramolecular chemistry to mimic biological systems: cyclodextrins as enzyme mimics, ion channel mimics, supramolecular catalysis etc.

Examples of recent developments in supramolecular chemistry from current literature

Text Books:

1. J.-M. Lehn; Supramolecular Chemistry-Concepts and Perspectives (Wiley-VCH, 1995)
2. P. D. Beer, P. A. Gale, D. K. Smith; Supramolecular Chemistry (Oxford University Press, 1999)
3. J. W. Steed and J. L. Atwood; Supramolecular Chemistry (Wiley, 2000)

CY 6106 - Organometallic Chemistry for Organic Synthesis

Review of formalisms such as oxidation state, 18-electron rule, classes of ligands, structure and bonding. Review of reaction mechanisms, ligand substitution, oxidative addition, reductive elimination, migratory insertion, hydride elimination, transmetallation, nucelophilic and electrophilic attack on the ligands coordinated to metals.

Organo zinc and copper reagents, preparation using transmetallation, functionalized zinc and copper reagents, synthetic applications in conjugate addition and allylic and propargylic substitution reactions.Organo tin reagents, hydrostannation reaction and synthetic utility of vinylstannanes and allylstannanes in addition and substitution reactions. Organoboron and aluminium reagents, alkyl and aryl derivatives, synthesis and examples of applications in C-C bond forming reactions. Organotitanium and zirconium reagents, metallocene complexes in C-C bond forming reactions. Addition to enynes and diynes, hydrozirconation, metallocycle formation and their synthetic utility.

Metal (W, Cr, Rh, Ru, Mo) carbene complexes, Fischer, Schrock and Grubbs type carbene complexes, comparison of their stability and reactivity, reactions of Fischer carbene complexes and their synthetic utility, Dötz reaction, simple and cross metathesis reactions, ring opening, ring closing metathesis in organic synthesis, examples from macrocycles synthesis. Copper and rhodium based carbene and nitrene complexes, cyclopropanation, Rh catalysed C-H insertion and aziridination reactions including asymmetric version. Introduction to N-heterocyclic carbene metal complexes. Metal (Fe, Cr, Mo, Ni, Co, Rh) carbonyl compounds in organic synthesis. C-C bond forming. Cyclooligomerization of alkenes, enynes and alkynes, Vollhardt reaction.Carbonylation and decarbonylation reactions and hydroformylation reaction.

Metal (Fe, Pd) ene, diene and dienyl complexes, metal complexes as protecting groups, activation towards nucleophilic addition reaction and rules governing such additions, synthetic utility. p-allyl palladium, nickel and iron complexes, synthesis and their synthetic utility. Various Wacker type oxidation and cyclization reactions including asymmetric version. Metal (Co, Zr) alkyne complexes, protection of triple bond, C-C bond forming reactions such as Pauson-Khand reaction, alkyne cyclotrimerization and oligomerization reaction. Metal (Cr, Fe, Ru) arene complexes, synthesis and structure. Activation of arene nucleus and side chain. Nucleophilic substitution and addition of arene. Metal (Rh, Ir) catalyzed C-H activation reactions and their synthetic utility.

Text Books:

1. Schlosser, M., Organometalllics in Synthesis, A manual, John Wiley, New York, 1996.
2. Hegedus, L.S.; Transition metals in the synthesis of complex organic molecules, second edition, University Science, Book, CA, 1999.
3. Astruc, D.; Organometallic Chemistry and Catalysis, Springer Verlag, 2007.
4. Davies, S. G.; Organotransition metal chemistry: Applications to organic synthesis, Pergamon Press, New York, 1986.

CY 6107 - Heterocyclic Chemistry

Nomenclature and classification of heterocycles

Structure, preparation and reactions of a) heterocyclic analogues of cyclopropane, cyclobutane, cyclopentadiene and benzene containing one or more heteroatoms (azeridine, oxirane, thiirane, oxaziridine, azetidine, azetidinone, oxetane, oxetanone, thietane, pyrrole, furan, thiophene, 1,2- and 1,3-azoles, triazoles, pyridine, pyryliums, diazines, triazine and their oxy-derivatives); b) fused heterocycles containing one or more heteroatoms (indoles, benzofurans, benzothiophene, benzanellated azoles, quinolines, isoquinolines, benzopyrones)

Heterocycles in natural products, medicine and materials.

Text Books:

1. Joule, J. A. and Mills, K. Heterocyclic Chemistry, Fifth Edition, Wiley, 2010.
2. Gilchrist, T. L., Heterocyclic Chemistry, Prentice Hall, 1997.
3. Acheson, R. M. An Introduction to the Chemistry of Heterocyclic Compounds, 3rd Ed, Wiley India Pvt Ltd, 2008.
4. Eicher, T.; and Hauptmann, S.; The chemistry of Heterocycles, Wiley-VCH, Weinheim, 2003.

CY 6108 - Medicinal Chemistry

Concept and definition of Pharmacophore. Pharmacodynamics and Pharmacokinetics – . Drug targets: enzymes and receptors. Competitive, non-competitive and allosteric inhibitors, transition-state analogs and suicide substrates. Nucleic acids as drug targets: reversible DNA binding agents, DNA alkylating agents and DNA strand breakers. ADMET of drugs: Factors affecting Absorption, Distribution, Metabolism, Elimination and Toxicity.

Drug Discovery, Design and Development. Structure-activity relationships: Strategies in drug design. QSAR and combinatorial synthesis. Optimization of drug-target interactions and access to drug targets. Pro-drugs and drug delivery systems.

Illustration of drug development through specific examples: a) Antibacterials: sulfonamides and penicillins b) Antivirals: case studies with inhibitors of reverse transcriptase (nucleoside reverse transcriptase- and non-nucleoside reverse transcriptase inhibitors) and protease inhibitors. c) Anticancer agents: antimetabolite-based approaches, those which affect signaling pathways or structural proteins such as tubulin. Drug resistance, Drug synergism and combination therapy.

References:

1. Patric, G. L., *An Introduction to Medicinal Chemistry*. 3rd ed.; Oxford University Press: 2005.
2. Silverman, R. B., *The Organic Chemistry of Drug Design and Drug Action*. 2nd ed.; Academic Press: 2004.
3. Williams, D. A.; Lemke, T. L., *Foye's Principles of Medicinal Chemistry*. 5th ed.; Wolters Kluwer Health (India) Pvt. Ltd.: 2006.

CY 6109 – Photochemistry

Principles and concepts: An overview of: Laws of photochemistry, Beer-Lambert law, electronic energy levels, atomic and molecular term symbols, singlet-triplet state, intensity and strength of electronic transition, selection rules for electronic transition, Jablonski diagram and photophysical processes, Franck-Condon principle. Excited state lifetime, steady state and time resolved emission, factors affecting excited state energy: solvent effect, TICT.

Excited state kinetics, quantum yield expressions, excimer and exciplex, kinetics of luminescence quenching: static and dynamic, Stern-Volmer analysis, deviation from Stern-Volmer kinetics. Photoinduced electron transfer rates, free energy dependence of electron transfer on rate, Photoinduced energy transfer, FRET, rate and efficiency calculation of FRET.

Methods: Measurement of fluorescence and phosphorescence and lifetimes. Introduction to time-resolved techniques for absorption and emission measurements, detection and kinetics of reactive intermediates. Examples of low temperature matrix isolation of reactive intermediates.

Reactions: Photochemistry of alkene, *cis-trans* isomerization, photocycloaddition reactions of alkene, photochemical electrocyclic and sigmatropic reactions, di-pi-methane rearrangment, electron transfer mediated reactions of alkene. Photochemistry of carbonyl compounds, Norrish type I and type II reactions, enone and dienone cycloadditions. Photochemistry of aromatic systems, electron transfer and nucleophilic substitution reactions. Photochemistry of nitro, azo and diazo compounds. Photochemistry involving molecular oxygen, generation and reactions of singlet oxygen. Photo-fragmentation reactions (Barton, Hofmann-Loffler-Freytag)

Applications

Fluorescence based sensors – examples of molecular and supramolecular systems. Conversion of solar energy to chemical and other forms of energies, solar photovoltaic cell, basic principle and design of the cell.

References

1. Fundamental of Photochemistry, K. K. Rohatgi-Mukherjee, New Age International (P) Ltd., New Delhi, 1986.
2. Principles of Fluorescence Spectroscopy, 3rd Ed., J. R. Lakowicz, Springer, New York, 2006.
3. Fundamentals of Photoinduced Electron Transfer, G. J. Kavarnos, VCH publishers Inc., New York, 1993.
4. Molecular Fluorescence: Principles and Applications, B. Valeur, Wiley-VCH Verlag GmbH, Weinheim, 2002.
5. Modern Molecular Photochemistry of Organic Molecules, N. J. Turro, V. Ramamurthy, J. C. Scaiano, University Science, Books, CA, 2010.
6. Photochemical Synthesis, I. Ninomiya, T. Naito, Academic Press, New York, 1989.

CY 6110 - Stereoselective Synthesis of Natural Products

Broad classification of natural products. Isolation, biosynthesis and stereo/enantio-selective synthesis of representative examples from the domain of Alkaloids, Steroids, Terpenes, Hormones, Pheromones, Macrolides, Penicillins and Prostaglandins. Synthesis of lead molecules based on natural products for different therapeutic areas.

References:

1. Classics in Total Synthesis by K. C. Nicolaou & E. J. Sorensen, VCH, 1996.
2. Classics in Total Synthesis II, K. C. Nicolaou & S. A. Snyder, VCH, 2003.
3. The Logic of Chemical Synthesis by E. J. Corey & X-M. Cheng
4. Natural Products Chemistry & Applications, Bhat, S.V.; Nagasampagi, B. A. & Meenakshi, S Narosa Publishing House, 2009
5. Classics in Stereoselective Synthesis by Carreira, E. M.; Kvaerno, L, Wiley VCH, 2009

CY 6111 - Electron Spectroscopy

Photoelectric effect: Need for electron spectroscopy, basic principles of electron spectroscopy, classification of various spectroscopic techniques, history.Photoelectron spectroscopy: Electron energy analysis; photon sources -- UV, X-ray, synchrotron; vacuum - angular dependence - cross section and its determination; valence and core photoemission - Koopmans‘ theorem; final state effects; photoelectron diffraction; band structure- holography- circular dichroism - supersonic molecular beam spectroscopy - coincidence studies. Applications of photoelectron spectroscopy – catalysis, surface structure. Size dependence of electronic structureAuger electron spectroscopy: introduction - instrumentation - classification of various transitions - quantification - applications**.**

Electron energy loss spectroscopy: Franck and Hertz experiment -- instrumentation - selection rules-theory - studies on molecules - surface states - high resolution spectroscopy - adsorption and catalysis –applications.

Related techniques: Inverse photoemission - multiphoton ionization - electron momentum spectroscopy - photoionization-photodetachment - zero kinetic energy photoelectron spectroscopy - spin resolved photoemission - recent advances in instrumentation-brighter photon sources. Several of form of infra-red spectroscopy, viz., transmission, diffuse reflectance (DRIFT), reflection-absorption (RAIRS) and multiple internal reflection (MIR).

Text Books:

1. Stefan Hufner, Photoelectron Spectroscopy, Springer-Verlag, Heidelberg, 1995
2. P. K. Ghosh, Introduction to Photoelectron Spectroscopy, Wiley Interscience, 1983.
3. A. D. Baker and C. R. Brundle, Eds, Electron Spectroscopy, Vol. 1 - 4 Academic Press, 1978.
4. H. Ibach, Electron Energy Loss Spectroscopy, Springer Verlag, 1992.
5. D. Briggs and M. P. Seah, Editors, Practical Surface Analysis, 2nd ed. vols 1 & 2, Auger and x-ray photoelectron spectroscopy, John Wiley & Sons, 1990.

CY 6112 - Surface Chemistry and Catalysis

Surface phenomena: Structure of clean surfaces; Notation of surface structure; Structure of adsorbate layers; Stepped surfaces; Surface relaxation and reconstruction; Dynamics and energetics of surfaces.

Heterogeneous Catalysis: Adsorption isotherms, surface area, pore size and acid strength measurements; Porous solids; Catalysis by metals, semiconductors and solid acids; Supported metal catalysts; Catalyst preparation, deactivation and regeneration. Model catalysts: Ammonia synthesis; Hydrogenation of carbon monoxide; Hydrocarbon conversion.

Instrumental methods of catalyst characterization: Diffraction and thermal methods; spectroscopic and microscopic techniques.

References:

1. A. Zangwill, Physics at Surfaces, Cambridge Univ. Press, 1988.
2. B. Gates, Catalytic Chemistry, Wiley, 1992.
3. A.W. Adamson, A.P. Gast, Physical Chemistry of Surfaces, Wiley, 1997.
4. J. M. Thomas and W.J. Thomas, Principles and Practice of Heterogeneous Catalysis, Wiley-VCH, 1997.
5. K.W. Kolasinski, Surface Science: Foundations of Catalysis and Nanoscience, Wiley, 2002.
6. D.K. Chakrabarty and B. Viswanathan, Heterogeneous Catalysis, New Age, 2008.
7. G.A. Somorjai, Y. Li , Introduction to Surface Chemistry and Catalysis, Wiley, 2010.
8. Physical chemistry of surfaces by Arthur W. Adamson 1990
9. Chemical kinetics and catalysis by R.I. Masel, Wiley-Interscience, 2001.
10. The chemical physics of surfaces by Roy S. Morrison, S. Roy, 1990.
11. An introduction to chemisorption and catalysis by metals", R.P.H. Gasser, 1985.
12. Modern techniques of surface science by D.P. Woodruff, T.A. Delchar, Cambridge Univ. Press, 1994.
13. Introduction to Scanning Tunneling Microscopy by C. J. Chen, Oxford University Press, New York, 1993.

CY 6113 - Chemistry of Macromolecules

Basic concepts - classification, nomenclature, molecular weights, molecular weight distribution, glass transition, degree of crystallinity, morphology, and viscosity-molecular weight, mechanical property - molecular weight relationships.

Molecular weights and Methods of determination, molecular weight distribution, size and shape of macromolecules. Intrinsic viscosity, Mark-Houwink relationship.

Chain structure and configuration, conformation, size of an ideal chain (freely jointed chain and other models), Real chains, Flory theory.

Thermodynamics of polymer solutions.

Molecular motion (self-diffusion, hydrodynamic radius, Rouse Model, Zimm Model, entangled polymer dynamics and de Gennes reptation model).

Glass transition temperature – elementary theories and methods of determination. Variation of glass transition with structure.

Rubber elasticity - concepts, thermodynamic equation of state. Elementary theories of viscoelasticity (Maxwell, Voight).

Mechanisms and Methods of Polymerization - Step (condensation) polymerization - Description - Reactivity Functional Groups - Kinetic and thermodynamic considerations - Molecular weight distribution. Chain polymerization, controlled radical polymerizations (INIFERTER, ATRP, RAFT, SET). Living Polymerizations. Ziegler-Natta and metathesis polymerizations.

Selected Applications

Text Books:

1. R. J. Young and P. A. Lovell, Introduction to Polymers, 2nd Edition, Chapman and Hall, 2002.
2. F. W. Billmeyer, Textbook of Polymer Science, 3rd Edition, John Wiley, 1994.
3. V. R. Gowariker, N. V. Viswanathan, Jayadev Sreedhar, New Age International (P) Ltd, 2005.
4. G. Odian, Principles of Polymerization, Fourth edition, Wiley-Interscience, 2004.
5. L. H. Sperling, Introduction to Physical Polymer Science, Wiley- Interscience, 1986.
6. M. Rubinstein and R. A. Colby, Polymer Physics, Oxford University Press, 2003.

CY 6114 - Chemical and Electrochemical Energy Systems

Available energy options, their advantages and disadvantages. Environmental effects, comparative evaluation of energy options and energy needs**.**

Fossil fuels: petroleum, natural gas and coal - Origin, processing and production of value added products - available current conversion technologies.

Nuclear Energy: Principles of Fission - Fission reactors, U enrichment and processing of spent fuels. Nuclear reactor kinetics and control - nuclear fusion - magnetic and other confinement - evaluation of the option of nuclear energy.

Electrochemical power sources - theoretical background on the basis of thermodynamic and kinetic considerations.

Primary cells - various types, especially magnesium and aluminium based cells - magnesium reserve batteries.

Secondary cells: classification based on electrolyte type, temperature of operation on the basis of electrodes - chemistry of the main secondary batteries - Batteries for electric vehicles - present status.

Fuel cells - classification - chemistry of fuel cells - detailed description of hydrogen/oxygen fuel cells - methanol - molten carbonate solid polymer electrolyte and biochemical fuel cells.

Solar energy conversion devices - photovoltaic cells - photoelectrochemical cells - semiconductor electrolyte junctions photocatalytic modes for fuel conversion process - photobiochemical options.

Hydrogen as a fuel - production (thermal, electrolysis, photolysis and photoelectrochemical) storage and applications of hydrogen storage.

Other methods of energy conversion: processes especially in the form of storage as chemical energy.

Text Books:

1. C. A. Vincent Modern Batteries, Edward Arnold, 1984.
2. R. Narayanan and B. Viswanathan, Chemical and Electrochemical energy systems, Orient Longmans, 1997.
3. K. Sriram, Basic Nuclear Engineering, Wiley Eastern, 1990.
4. A. S. J.. Appleby and F. K. Foulkes, Fuel cell Hand Book, Von Nostrand Reinhold, 1989.
5. D. Linden, Hand book of batteries and Fuel cells, McGraw Hill Book Company, 1984.
6. T. Ohta, Solar Hydrogen energy systems, Peragamon Press, 1979.
7. M. Gratzel, Energy Resources through photochemistry and catalysis, Academic Press, 1983.
8. T. Ohta, Energy Technology, Sources, Systems and Frontiers conversions, Pergamon, 1994.
9. J. G. Speight, The chemistry and technology of petroleum, Marcel Dekker Inc. (1980).

CY 6115 - Chemistry of the Earth's atmosphere

Introduction to the Earth's Atmosphere:

Evaluation of the Earth's atmosphere – Layers of atmosphere – Pressure and Temperature variations – Scaling of atmospheric processes.

Role of Chemical Compounds on Ozone budget:

Chemical composition of the Earth's atmosphere – Compounds containing Sulfur, Nitrogen, Carbon, Halogens – Atmospheric Ozone – Ozone loss – role of the chemical compounds – Atmospheric lifetimes – Theories – Determination of the lifetimes – Laser Induced Fluorescence Studies (LIF measurements) – Cavity Ring Down method; Radicals in the Earth's atmosphere – Ozone generation – Global warming – Global Warming Potential (GWP) – Ozone Depletion Potential (ODP)

Chemistry of Troposphere and Stratosphere:

Troposphere – Chemistry of hydroxyl radicals – Photochemical cycles of NO_2, NO and O_3 – Chemistry of NO_X and carbon monoxide – Methane – Tropospheric reservoir molecules – H_2O_2, CH_3OOH, HONO, PAN, Role of VOC and NO_x in the ozone formation – Chemistry of VOCs – sulfur compounds – nitrogen compounds;

Stratosphere – Chapman mechanism – HO_X cycle – Halogen cycles – Antarctic ozone hole – Polar stratospheric clouds – Heterogeneous stratospheric chemistry – Global sulfur and carbon cycles – Role of H_2O in both troposphere and the stratosphere.

Atmospheric Radiation and Photochemistry:

Radiation – Terrestrial and solar radiation – Energy balance for Earth and Atmosphere

– Radiative flux – Actinic flux; Photochemistry – Absorption of radiation by atmospheric gases – Absorption by O_2 and O_3 – Photolysis rate as a function of altitude

– Photodissociation of O_3, NO_2.

Aerosols and Other Physical Processes:

Aerosols – formation – Size distribution – Chemical composition – thermodynamics of aerosols; Nucleation – Classical theory of homogeneous nucleation – Experimental measurement of nucleation rates – heterogeneous nucleation; Wet and dry deposition.

Text Books:

1. Atmospheric chemistry and Physics by John H. Seinfeld, Spyros N. Pandis; Second edition, John Wiley, 1997.

2. Introduction to Atmospheric Chemistry by Daniel J. Jacob, Princeton University Press, 1999.

3. Introduction to Atmospheric Chemistry by Peter V. Hobbs, Cambridge University Press, 1st edition, 2000.

4. Chemistry of Atmospheres: An Introduction to the Chemistry of the Atmospheres of Earth, the Planets, and Their Satellites by Richard P. Wayne, Cambridge University Press, 3rd edition, 1991.

CY 6116 - Advanced Solution Thermodynamics

Ideal and non-ideal solutions, activity and activity coefficients, mixing and excess properties of liquid-liquid mixtures. Theories of solutions of electrolyte and non-electrolyte liquids: van Laar theory, van der Waals theory, Scatchard-Hildebrand theory, Lattice theory, Prigogine Cell theory, Flory equation of state theory, Prigogine-Flory-Patterson theory, Extended Real Associated Solution model and Kirkwood-Buff theory.

Modern experimental techniques: determination of vapour-liquid equilibrium by static and dynamic methods, heat capacity and heat of mixing by calorimeters, and determination of volumetric, transport, acoustic and optical properties of liquid-liquid mixtures. Thermodynamic relations of excess Gibbs energy, excess entropy, excess enthalpy, excess volume, viscosity deviation, excess heat capacity and excess compressibility. Partial molar properties, their physical significance and methods of their determination. Study of non-ideal behaviour of various types of solutions: nonpolar + nonpolar, polar + nonpolar, polar + polar, and mixtures with hydrogen-bond formation and charge transfer complexes; interpretation in terms of molecular interactions.

Empirical and semi-empirical formulas, theoretical expressions, correlations, group contribution methods and computational models for the prediction of thermodynamic properties of liquids and liquid mixtures.

Text Books:

1. Prausnitz J. M., Lichtenthaler R.N., Azevedo E.G., Molecular Thermodynamic of Fluid-Phase Equilibria, (Prentice Hall, 3rd edition, 1998).
2. Rowlinson J.S., Liquid and Liquid Mixtures, (Springer; 1st edition, 1995).
3. Acree W.E., Thermodynamic Properties of Nonelectrolyte Solutions, (Academic Press, 1984).
4. J. Bevan Ott, Juliana Boerio-Goates, Chemical Thermodynamics: Advanced Applications, (Academic Press, 1st edition, 2000).
5. Prigogine, The Molecular Theory of Solutions, (North Holland Publishing Co. Amsterdam 1957).
6. Arieh Ben-Naim, Molecular Theory of Solutions, (Oxford University Press, USA, 2006).

CY 6117 - Advanced Optical Spectroscopy

Overview of basic concepts: Light-matter interaction, Einstein coefficients, introduction to lasers, transition dipole moment, selection rules for electronic transitions, Jablonskii diagram, fluorescence and phosphorescence, kinetics of unimolecular and bimolecular processes.

Advanced concepts: Theory of nonradiative transitions, spin-orbit coupling and singlet-triplet transitions, polarized light absorption and emission: fluorescence anisotropy, solvation dynamics, energetics and dynamics of bimolecular processes like excimer and exciplex formation, resonance energy transfer, mechanisms of fluorescence quenching, introduction to non-linear spectroscopy.

Techniques and instrumentation: Uv-Vis spectrophotometry, steady-state fluorimetry, lasers as excitation sources, time-resolved fluorimetry, transient absorption spectroscopy, surface plasmon spectroscopy, evanescent wave spectroscopy, multiphoton spectroscopy, single-molecule spectroscopy, fluorescence correlation spectroscopy.

Applications: Microscopy (optical, phase-contrast, confocal, FLIM). Applications in biology and analytical chemistry.

Text Books:

1. Modern Spectroscopy, J M Hollas, John Wiley & Sons, 4th Edn, 2004
2. Modern Optical Spectroscopy, William W Parson, Springer, Student Edn, 2009
3. Fundamentals of Photochemistry, K K Rohatgi-Mukhejee, Wiley Eastern Ltd, 1992
4. Principles of Fluorescence Spectroscopy, J R Lakowicz, Springer, 3rd Edn, 2006
5. Laser Spectroscopy- Basic concepts and instrumentation – W. Demtroder (Springer 3rd edition, 2004)

CY 6118 - Experimental Methods in Chemistry

Vacuum and Gas Pressure: Concepts of vacuum (Low, medium, high and ultra-high vacuum; vacuum pumps and gauges; pressure measurements;); kinetic theory concepts (molecular density; mean free path of particles in the gas phase; incident molecular flux on surfaces; gas exposure; sticking coefficient; surface coverage; variation of parameters with pressure).

Over layers and Diffraction: Two-dimensional lattice; reciprocal space; over layer structure; low energy electron diffraction (LEED).

Imaging and Depth Profiling: Basic concepts in surface imaging; secondary electron microscopy (SEM); secondary Auger microscopy (SAM); scanning probe microscopy (SPM); scanning tunneling microscopy (STM); transmission electron microscopy (TEM); surface imaging; depth profiling. Associated techniques of microscopy and spectroscopy.

Chemical Analysis: *Non-destructive techniques*: Wavelength and energy dispersive X-ray fluorescence spectroscopy (WDS and EDS); X-ray absorption spectroscopy (XANES and EXAFS); secondary ion mass spectrometry (SIMS); temperature programmed desorption (TPD); thermal desorption spectroscopy (TDS). *Destructive techniques*:

Atomic absorption spectroscopy (AAS); inductively coupled plasma-atomic emission spectroscopy (ICP-AES).

Electroanalytical Techniques: Voltametry; coulometry; amperometry; potentiometry; polarography; electrolytic conductivity; impedance spectroscopy.

Separation Methods: Normal and reversed phase liquid chromatography (NP- & RP-LC); Gas Chromatography (GC); GC-MS; High Performance Liquid Chromatography (HPLC)**;** Size-Exclusion Chromatography (SEC); Ion Chromatography (IC).

Reading assignments on: Quantitative measurements: Limit of detection, limit of quantification, sensitivity, calibration, interferences, sampling; Laboratory practice, laboratory automation.

Text Books:

1. R. Wiesendanger, *Scanning Probe Microscopy and Spectroscopy,* Cambridge University Press, 1994.
2. Frank A. Settle, Handbook of instrumental techniques for analytical chemistry, Prince Hall, New Jersey, 1997.
3. K. W. Kolasinski, Surface science: Foundations of catalysis and nanoscience, John Wiley and Sons, West Susses, 2002.
4. D. A. Skoog, D. M. West, F. J. Holler and S. R. Couch, Fundamentals of analytical chemistry. Brooks/ColeCengage learning, New Delhi, 2004.
5. P. Atkins and J. de Paula, Atkins‘ physical chemistry, 8th Ed., Oxford University Press, New Delhi, 2008.
6. T. Pradeep, Nano: The essentials, McGraw-Hill Education, New Delhi, 2010.
7. F. Scholz, Electroanalytical Methods, Springer, 2nd Ed., 2010.

CY 6119 - Group Theory and Molecular Spectroscopy

The complete nuclear permutation and permutation – inversion group, molecular symmetry groups, Double groups, point group symmetry, representation and character tables. The molecular Hamiltonain and its symmetry. Nuclear spin statistics. Examples of application of MS group to non-rigid molecules and molecular complexes.

General formalism for molecular Hamiltonians in curvilinear coordinates –Podolsky transformation, Echart-Sayvetz. Rotational – vibrational Hamiltonians with emphasis on coupling terms for semirigid diatomic and polyatomic molecules. The Wilson – Howard – Darling - Dennison and the Watson Hamiltonians. Contact transformation and the derivation of effective rotational Hamiltonians for vibrational degrees of freedom. Coriolis and centrifugal coupling. Advanced theory of line intensities for infrared and Raman Spectra. Symmetry of ro-vibronic wave function and introduction to vibrational – rotational spectra of non-rigid molecules and molecular complexes

Text Books:

1. Bunker, P.R. and Per Jensen, Molecular Symmetry and Spectroscopy, NRC Press, Ottawa, Canada, 1998.
2. Wilson, Jr.E.B., Decius, J.C. and Cross, P.C., Molecular vibrations, Dover,New York, 1980
3. Allen, Jr.H.C and Cross,P.C., Molecular Vib-Rotors: The Theory and Interpretation of High Resolution Infrared Spectra, Wiley, New York, 1963.
4. Papousek, D. and Aliev, M.R. Molecular Vibrational-Rotational spectra, Elsevier, 1982.
5. Bishop,D.M., Group Theory and Chemistry, Dover, New York, 1993.
6. Bhagavantam, S. and Venkatarayudu, T., Theory of Groups and its applications to Physical Problems, Academic Press, New York, 1969.

CY 6120 - Molecular and Statistical Reaction Dynamics and Scattering Statistical dynamics:

Transition state Theory – Thermodynamics formulation; micro-canonical and variational transition state theory; flexible transition states. Unimolecular reaction dynamics, RRK and RRKM models, thermal activation, density of state. State preparation and intra molecular vibration energy distribution; stochastic master equation approach dynamical approaches to unimolecular reaction rates.

Electron transfer reactions, Marcus model. Statistical density operator for molecular states and the equations of motion for chemical system; Chemical reactions in solutions, diffusion equation, Kramer‘s and Grote –Hynes models. Quantum theory of reaction rates – flux-flux correlation function approach. Kubo formalism Quantum transition state theory.

Molecular dynamics:

Potential energy surface, bimolecular reaction, elementary quantum dynamics. Microscopic reversibility and detailed balance. Different forms for intermolecular potentials. Statistical sampling for simulations. The Metropolis Monte Carlo method; finite difference methods such as verlet algorithm and predictor-corrector methods. Introduction to quantum Monte Carlo. Procedure. Introduction to time-correlation and autocorrelation functions.

Molecular Scattering (elementary aspects only):

Bimolecular collisions, collision number two-body classical scattering. Cross sections, intermolecular potentials, import parameter principle of microscopic reversibility. Quantum theory of scattering: particles in central potentials partial waves, Born approximation optical theorem. Formal time independent scattering theory. The S matrix. The Lippmann – Schwinger equation – for structureless particles. Rate of change of observables, collision rates in ensembles and the relaxation equation. The wave (Moller) operator and time dependent collision theory, time reversal and reciprocity

Text Books:

1. Steinfeld, J. I., Francisco, J.S. and W.L., Chemical Kinetics and Dynamics, Prentice Hall, New Jersey, 1998.
2. Baer, T and Hase, W.L., Unimolecular Reaction Dynamics: Theory Experiments, Oxford University Press, Oxford, 1996.
3. Allen, D.J. and Tildesley, M.P., Computer Simulation in Liquids, Oxford University Press , U.S.A., 1996.
4. Haile, J.M., Molecular Dynamics Simulations, Wiley, U.S.A., 1997.
5. Taylor, J.R., Scattering Theory: The Quantum Theory of Non-relativistic Collisions, Dover, New York, 2006.
6. Levine, R.D., Molecular Reaction dynamics, Cambridge University Press, 2006.
7. Levine, R.D., Quantum Mechanics of Molecular Rate Processes, Dover, New York, 1999.
8. W.H. Miller, in Dynamics of Chemical Reactions, ed.R.E. Wyatt, Marcel-Dekker, U.S. A., 1998.

CY 6121 - Advanced Electronic Structure and Density Functional Theory for Molecules

The Hartree – Fock method, derivation and interpretation of HF equations, Roothaan equations. Basis sets – Gaussian and Slater type orbitals Independent electron pair approximation, coupled cluster approximation, cluster expansion of a wave function. Configuration interactions. Many body approach Moller – Plesset perturbation theory. Diagrammatic representation, one particles perturbation. Static electric and magnetic properties of molecules and multiple expansions.

Density matrices, reduced density operators, Thomas – Fermis model, Hobenberg – Kohn theorem. Chemical potential. Hardness and softness, Kohn – Sham method – basic principles, local density and Xa approximation, spin density functional and local spin density approximation. Exchange correlation energy-functional. Introductory account of popular functionals – B3LYP and MPW1PW91.

Simple applications of density functional theory for electronic structure.
Or
Electrons in the periodic lattice. Bloch states and Wannier functions.

Dynamics of interacting quantum spin systems in the presence of external fields – Ising and Heisenberg Hamiltonians. Theory of Ferromagnetism. Quantum phase transitions.

Text Books:

1. Szabo, A. and Ostlund, N.S., Quantum Chemistry, Dover, New York 1996.
2. Helagaker, T., Jorgenson, P. nad Oslen. J. Molecular Electronic Structure Theory, John Wiley & Sons, New York, 2000.
3. Cook, D.B., Handbook of Computational Quantum Chemistry, Dover, New York, 2005.
4. Parr, R.G. and Yang, W. Density Functional Theory of Atoms and Molecules, Oxford University Press, Oxford, 1989.
5. Mc Weeny, R., Methods of Molecular Quantum Mechanics, Academic Press, San Diego, 2001.
6. Koch, W.C. and Holthausen, M.C., A Chemist‘s Guide to Density Functional Theory, Wiley-VCH, Germany, 2000
7. Aurerbach, A. Interacting Electrons and Quantum Magnetism, Springer, 1994.
8. Mattis, D.C., Theory of Magnetism, World Scientific, Singapore, 2006
9. Van Vleck, J. H., theory of Electric and Magnetic Susceptibilities, Oxford, U.S.A., 1932

CY 6122 - Numeric Methods for Computational Chemistry

Programming Tools:

Introduction to C Programming:

Variables and arithmetic expressions, Symbolic Constants, Input and Output, Arrays and functions, Data types, arithmetic, relational and logical operators, simple control-flow statements, classes and modules and ability to write small programs in C for computations such as function evaluation and elementary linear algebra.

Or

Introduction to FORTRAN programming:

Constants and variables, arithmetic, input and output statements, control statements (Do, Go To If statements) , arrays, subprograms (Functions and subrountines), modules and ability to write small programs for computations such as function evaluation and elementary linear algebra.

Numerical Analysis:

Numerical interpolation, Polynomial and cubic spline interpolation, extrapolation of data. Numerical first and second derivatives, error analysis and Richardson‘s method.

Non-linear equations and roots of polynomials, Newton-Raphson method, secant method and Bairstow method. Numerical integration: Gaussian quadrature—Gauss-Hermite and Gauss-Legendre intervals; applications form quantum chemistry with Gaussian orbitals

Linear algebra: Householder reduction and LU decompositions, matrix inversion, determinant evaluation and eigenvalues and eigenvectors of hermitian (complex) and symmetric (real) matrices. Iterative methods for large-scale eigen value problems – Lanczos recursion, Arnoldi algorithm and Davidson‘s method. Or Fast Fourier transform, Fourier transform of real data in two and three dimensions. Introduction to finite basis representation and discrete variable. Simple applications from computational chemistry and spectroscopy.

Text Books:

1. Press, W.H., Teukolsky, S.A., Vetterling W.T.and Flannery, B.P., Numerical Recipes; The Art of scientific Computing, Cambridge University Press, New York, 2007.
2. Lanczos, C., Applied Analysis, Dover New York, 2010.
3. Koonin, S.E. and Meredith , D.C., Computational Physics , Fortran Version, Version, Westview Press, U.S.A., 1998.
4. Kerninghan, B.W. and Ritchie, D.M., The C Programming Language, Prentice Hall, New Jersey, 1988.
5. Rajaraman , V., Computer Programming on Fortran 90 and 95, Prentice-Hall of India, New Delhi, 2006.
6. Light, J.C. and Carrington Jr., T., Discrete Variable Representations and Their Utilization, Advances in Chemical Physics, Volume 114, pp 263-310, 2000.

CY 6998 - Electrochemical Approaches to Functional Supramolecular Systems

Objectives:

The course embodies a combined approach of supramolecular chemistry with electrochemistry that has produced a wealth of interesting functions and devices and their practical applications in energy conversion technology, advanced materials and diagnostics. The objective of the course is to bring forth the current electrochemical research applied to multi-component chemical systems with a special attention to properties and functions. The course, structured for ~ 40 lectures during an even semester, will cater to Ph. D as well as M. Sc / M. Tech graduate students (in a limited sense to B. Techs) who wish to explore the frontiers of electrochemistry with materials and nanosciences.

The essential features of the syllabus are the following:

(1) Analytical electrochemistry
(2) Bio-electrochemistry
(3) Electrochemical materials science
(4) Electrochemical energy conversion and storage

Detailed Syllabus:

Fundamental Concepts in Analytical Electrochemistry

Mass transport, Linear diffusion, Fick's laws and diffusion coefficient, The charged interface, Potential step and potential sweep experiments, Reactions controlled by rate of electron transfer and activated complex theory

Electrode Types and Study of Electrode Reactions:

Carbon electrodes, Semiconductor film electrodes, Microelectrodes, Ultra-micro electrodes, Ion-selective electrodes, Porous electrodes and non uniform reaction rates, Hydrodynamic/Rotating disk electrodes, Semiconductor electrodes and electrical capacitance

Cyclic voltammetry in reversible, quasi-reversible and irreversible systems, Study of reaction mechanisms, Surface modification in charge transfer and interfacial activity Electron transfer in DNA and biosystems

Spectro-Electrochemical and Spectroscopic Techniques:

Impedance Spectroscopy, Scanning Electrochemical Microscopy, Electrochemical AFM and STM, , Electrochemical Quartz Crystal Microbalance

Electrochemical Materials and Sensors:

Electroactive Fullerenes, Carbon Nanotubes, Biomolecules, Controlled Potential Techniques, Electrochemical synthesis of nanomaterials, nanowires and conducting polymers, Functional nanoparticles as catalysts and sensors, MOSFETS and ISFETS, Solid state molecular devices

Electrochemical Energy Systems:

Photo-electrochemistry, Monitoring photolytic intermediates, Electroluminescence and devices and sensors, Electro - chemiluminescence, Digital simulation of electrochemical problems, Sample BASIC programs

Fuel cells: Electrode materials, Diagnostic tools in fuel cell research, Determination of injection efficiency and electron diffusion length under steady state condition, Small-amplitude time-resolved methods, Organic solar cells

Recommended Books:

1. Allen J. Bard and Larry R. Faulkner, Electrochemical Methods: Fundamentals and Applications, 2nd edition 2001, John Wiley & Sons
2. Allen J. Bard (Ed), Electroanalytical Chemistry, Vol.13, Plenum Press 1983
3. Joseph Wang, Analytical Electrochemistry, 3rd edition 2006, John Wiley & Sons
4. Paola Ceroni, Alberto Credi and Margherita Venturi (Ed), Electrochemistry of Functional Supramolecular Systems, 2010, John Wiley & Sons
5. Kosuke Isutzu, Electrochemistry in Non-aqueous Solutions, Wiley – VCH Verlag GmbH & Co. 2002
6. K. Kalyanasundaram (Ed), Dye-Sensitized Solar Cells, EPFL Press, 1st Edition 2010(ISBN 978-2-940222-36-0)
7. J. Newman, Electrochemical Systems, Wiley-Interscience, 3rd edition 2004

CY 6123 - Asymmetric Organic synthesis

Course Objectives*:* Learn various asymmetric transformations and employ such reactions in asymmetric organic synthesis of important chiral molecules.

Learning Outcome: At the end of the course, the learners should be able to:

Apply *asymmetric transformations in a logical manner for the synthesis of chiral molecules.*

Course Contents:

Stereoselective reactions: Classification, importance and advantages; diastereoselective reactions.

Asymmetric synthesis: Importance, classification and principle; modes of asymmetric induction

Metal catalyzed asymmetric enantioselective oxidation, reduction, C-C bond forming reactions, allylic substitution, cyclization, and other important reactions.

Chiral organocatalysts including phase transfer catalysts and hydrogen-bonding catalysts, and supported chiral catalysts.

Kinetic resolution, parallel kinetic resolution, dynamic kinetic resolution and dynamic thermodynamic resolution.

Chiral poisoning, chiral activation, desymmetrization, nonlinear effect, autocatalysis, auto induction, double diastereoselection and remote chiral induction in asymmetric synthesis

Determination of optical purity using NMR, GC and HPLC techniques including principles, determination of absolute configuration by NMR and X-Ray crystallography.

Application of asymmetric synthesis in the industrially relevant molecules such as L-DOPA, (S)-metolachlor, carbapenem and menthol.

Text Books:

1. Stereoselectivity in organic synthesis, G. Procter, Oxford Chemistry Primers, 2007.
2. Fundamentals of asymmetric catalysis, P.J.Walsh and M.C. Kozlowski, University science books, USA, 2009.
3. Catalytic Asymmetric Synthesis, 3rd ed,Ed: I. Ojima, John Wiley & Sons, New Jersey, 2010.
4. Comprehensive Asymmetric Catalysis I-III; Editors: Eric N. Jacobsen, Andreas Pfaltz, Hisashi Yamamoto; Springer-Verlag Berlin Heidelberg, Germany, 1999.
5. Asymmetric Synthesis – The Essentials, Eds.: M. Christmann and S. Brase, Wiley-VCH Verlag GmbH, Weinheim, 2007.

CY 6124- Organic Photochemistry: Principles and Applications

Course objectives: Learn the fundamental ideas of photochemical excitation/de-excitation events, and the molecular events that can intervene at different levels and their applications.

Learning Outcomes: *At the end of the course, the learners should be able to:*

Predict *the course of an organic photochemical reaction and identify the product with the type of functional group present on the molecule*

Apply *photochemistry concepts, plan and program molecules for photochemical application of specific interest*

Appreciate *the photochemical phenomena by light and be able to* ***design*** *and* ***practically carry out*** *simple photochemical reactions*

Course Contents:

Fundamentals – Energy and electronic spin states – spectroscopic transitions – photophysical processes, fluorescence and phosphorescence – energy transfer and electron transfer, and properties of excited states – reaction mechanisms Experimental Techniques – Photochemistry of olefins, carbonyl compounds, aromatic molecules – nitrogen containing compounds (nitro, azo, and diazo compounds) – molecular oxygen – photofragmentation and elimination reactions – photolytic deprotection and activation of functional groups – electron transfer reactions – applications to organic synthesis

Supramolecular photochemistry – Photochemistry in organized and constrained media

– Organic photoresponsive materials

Some applications in biochemistry, biology, medicine and technology.

Text Books:

1. Modern Molecular Photochemistry by N. J. Turro, University Science Books, US; 1991
2. Modern Molecular Photochemistry of Organic Molecules, N. J. Turro, V. Ramamurthy, and J. C. Scaiano, University Science Books, US; 2010.
3. Organic Photochemistry by J. M. Coxon and B. Halton, Cambridge University Press, New York;1974.
4. Organic Photochemistry: Principles and Applications by J. Kagan, Academic Press, London; 1993.
5. Photochemistry and Photophysics by V. Balzani, P. Ceroni, and A. Juris, Wiley-VCH, Verlag GmbH & Co; 2014.

CY 6125- Functional Organic Materials

Course objectives*:* Learn the basic theory and principles for the design of functional organics, particularly, organic electronic, photonic and energy materials as well as molecular machines.

Learning Outcome:

At the end of the course, the learners should be able to:

Express *clearly the fundamental mechanism behind various functional devices*

Correlate *the design, structure and functional aspects of various organic molecules*

Plan *and* ***design*** *new organic molecules based on the acquired knowledge for a specific function*

Course Contents:

Organic Electronic Materials: Basic theory and design of Molecular wires, Resistors, Diodes, Transistors/OFETs, and OLEDs - Introduction to various device configurations and working principles

Organic Photonic Materials: Basic theory and design of molecules for Organic solar cells – Various approaches and introduction to some device aspects – Molecules for NLO and imaging – Molecular switches, Motors and Memories – Chirooptical materials and Photorefractive materials

Organic Energy Materials: Basic theory and design of Organic Flow Batteries for Energy Storage applications – High energy materials – Covalent Organic Frameworks

Organic Molecular Machines: Types – Design, synthesis, and function – Examples

Miscellaneous Materials: Basic theory and design of materials for Organogels, Organic Sensors and Logic Gates, Organic Magnets, Organic Superconductors, Organic Thermoelectrics

Text Books:

1. Functional Organic Materials by T. J. J. Müller and U. H. F. Bunz, Wiley-VCH, 2007
2. Introduction to Organic Electronic and Optoelectronic Materials and Devices by Sam-Shajing Sun, Larry R. Dalton, CRC Press, 2008
3. Organic Electronics Materials and Devices by S. Ogawa, Springer, 2015
4. Electronic Processes in Organic Semiconductors: An Introduction by A. Kohler and H. Bassler, Wiley-VCH, 2015
5. Organic Optoelectronics by Wenping Hu, John Wiley and Sons, 2013
6. Molecular Machines by T. Ross Kelly, Topics in Current Chemistry (Springer), 262, 2005
7. A Journey Through the World of Molecular Machines by C. Davis, Create Space, 2010
8. Molecular Machines and Motors: Recent Advances and Perspectives by A. Credi, S. Silvi and M. Venturi, Topics in Current Chemistry (Springer), 354, 2014
9. Redox-Flow Batteries: From Metals to Organic Redox-Active Materials by J. Winsberg et al. *Angew. Chem. Int. Ed.* 2017, *56*, 686-711.

CY 6126- Green Organic Synthesis: Principles and Applications

Course Objectives: Learn the importance of minimizing waste, saving power and doing organic synthesis according to the principles of green chemistry

Learning outcomes: *At the end of the course, the learners should be able to:*

Create *awareness for reducing waste, minimizing energy consumption in organic synthesis.*

Implement *techniques of green synthesis in organic reactions*

Course Contents:

Green Chemistry Definition, need for Green chemistry, evolution of Green Chemistry, principles of Green Chemistry.

Classification of organic reactions under Green chemistry principles: a) Atom economic and non-toxic byproduct reactions: rearrangements, addition reaction, condensations, cascade strategies under catalysis, b) atom uneconomic reactions: substitutions, eliminations, Wittig reactions, degradation reactions

Green Strategies and techniques for Organic Synthesis: use of Microwave, Sonochemsitry, Ball mill technique, electrochemical reactions, photochemical reactions,

Catalysis: Principles of various catalysis techniques in terms of Green Organic Synthesis

i) Homogeneous, ii) Heterogeneous, iii) bio (enzyme) catalysis, iv) catalysis with non-toxic metals (Ca, Fe, Co, etc.), v) solid supported catalysis, vi) metal free/organocatalysis, vii) Visible light catalysis viii) phase transfer catalysis
Alternative/Green Solvents for Organic Synthesis i) Water, ii) Ionic liquids, iii) Supercritical liquids (SCL), iv) Poly(ethylene glycol) (PEG), v) Fluorous biphasic Solvents

Comparison of greenness of solvents

Understanding the role/effect of these solvents on organic reactions

Solvent Free Organic Synthesis

Reactions at Room Temperature

Applications of the Green strategies in Organic Synthesis

Comparing various organic reactions under classical conditions and Green conditions.

Text Books:

1. *Green Chemistry: An introductory text* by Mike Lancaster, RSC publishing, 2nd Edition, 2010.
2. *Green Chemistry: Theory and Practice* by Paul T. Anastas and John C. Warner, Oxford University Press, Oxford, 1998.
3. *Green Chemistry*: *Environment Friendly Alternatives* by Rashmi Sanghi and M M Srivastava, Narosa Publishing House, Delhi, 2003.
4. *Strategies for Green Organic Synthesis*, by V. K. Ahulwalia, Ane Books Pvt. Ltd. 1st Edition, 2012.

CY6127: Chemical Processes at Surfaces and Interfaces

Course objectives: To introduce the basic concepts of surface and interfacial chemistry. The subject is very diverse and interdisciplinary in nature. The topics cover the chemical processes that occur at solid-liquid, solid-gas and liquid-gas interfaces. The spectroscopy and microscopy methods to study the interfacial phenomena are also included in the syllabus for the benefit of chemistry, physics, engineering, and biology students.

Course Outcomes:
(i) Understand concepts of solid-liquid, solid-gas, liquid-gas interfaces
(ii) Apply fundamental principles of chemistry to chemical processes occurring at interfaces
(iii) Apply spectroscopic methods to study interfaces and interfacial phenomena

Course Contents:

Solids and solid surfaces : Crystalline surfaces, single crystal surface structures, surface relaxation, clean and adsorbate induced surface reconstructions, bimetallic and semiconductor surfaces, adsorbate overlayer structures and notations, thermodynamics of solid surfaces, surface energy and defects, surface diffusion, band structure of solids, Fermi energy and work function, density of states, quantum wires, nanostructures, and semiconductor quantum dots.

Energetics and kinetics of chemisorption, adsorption isotherms, measurement of heats of adsorption and isosteres, adsorption on porous materials, capillary condensation phenomenon and hysteresis. Kinetics of catalytic reactions on surfaces, structure sensitivity, chemisorbed molecular species on surfaces and Blyholder model of chemisorption bond, surface reaction mechanisms, oscillatory reactions. Friction and lubrication forces, polymer coated surfaces.

Spectroscopy methods to study solid surfaces, x-ray and UV photoemission spectroscopies, Inverse photoemission, Auger spectroscopy, LEED structure determination and RHEED, scanning probe microscopies (STM & AFM), Thermal methods, vibrational spectroscopy (RAIRS & HREELS, SERS).

Liquids and liquid surfaces: microscopic picture of liquid surface, surface and interfacial tension, Young-Laplace equation and its application, measurement of surface tension, Kelvin equation and capillary forces, nucleation and growth of aggregates, Ostwald ripening, surface excess and Gibbs adsorption isotherm. Organized molecular assemblies, surfactants and detergency, films of insoluble surfactants, Langmuir films and LB films, Langmuir trough, surface pressure-area relationships, self-assembling structures, soluble and insoluble monolayers, contact angle and wetting, capillary rise, dispersion, colloids, micelles (CMC), oil-water-surfactant phase diagram, vesicles, microemulsions, aerosols, surfactant and lipid membranes, liquid crystals, ionic liquids.

Electrode/electrolyte interface, electrochemical methods, cyclic voltammetry, electrochemistry on single crystal surfaces, shape-dependent electrocatalysis, semiconductor/electrolyte interface, spectroelectrochemistry.

Text Books:

1. Peter Atkins, J. De Paula, Atkins' Physical Chemistry 9th edition, 2010
2. H. Kuhn, H.-D. Forsterling, D.H. Waldeck, Principles of Physical Chemistry, Wiley 2nd edition, 2009
3. Physical chemistry – A molecular approach, D.A. McQuarrie and J.D. Simon, 1998
4. A.W. Adamson, A.P. Gast, Physical Chemistry of Surfaces, Wiley, 1997
5. G.A. Somorjai, Y. Li , Introduction to Surface Chemistry and Catalysis, 2nd edition, 2010
6. H.-J Butt, K. Graf and M. Kappal, Physics and Chemistry of Interfaces, 3rd edition, Wiley-VCH, 2013

Reference Books:

1. *Catalysis : Principles and applications*, Editors : B. Viswanathan, S. Sivasanker, A.V. Ramaswamy, Narosa Publishers, 2002
2. I. Chorkendorff, J.W. Niemantsverdriet, Concepts of Modern Catalysis and Kinetics, 2nd edition, Wiely-VCH, 2007
3. A. Zangwill, Physics at Surfaces, Oxford University Press, 1988
4. Jacob N. Israelachvili, Intermolecular and surface forces, 3rd edition, Elsevier-Academic Press, 2011

CY6128: Computational Quantum Chemistry and Molecular Simulations

Course Objectives:

- Introduce state-of-the-art molecular level computational methods using open source and commercial codes developed and used by researchers in chemical sciences worldwide.
- To provide hands-on training in the use of standard computer codes for a few selected topics in organic, inorganic, materials and physical chemistry.
- To provide hands-on training in molecular dynamics that would help the students use molecular modeling in protein-protein, protein-ligand and DNA-ligand interactions and other biomolecular simulations.

Course Outcomes:

- Students will be able to write simple programs/use existing free software codes in numerical linear programming package known as EISPACK for diagonalization of matrices, calculation of simple integrals using quadratures and do curve-fitting experimental data for specific least-squares models.
- Students will be able to use standard features of Gaussian 16 for calculating molecular structures, energies and spectroscopic properties of simple compounds important for a variety of applications
- Each student will perform one simulation/computation extensively, in his/her own areas of interest as a project and submit the results.

Course Topics:

Introduction to Numerical methods:

- Newton-Raphson method.
- Matrix diagonalization and Householder algorithm.
- Numerical quadrature (Gaussian and Gauss-Hermite).
- Elementary concepts in parallel computing/programming.

Classical and Statistical Mechanics based Dynamics Simulations

- Definitions of ensembles, introduction to Monte Carlo Method, sampling, Metropolis Algorithm, trial moves and application.
- Definition of force fields, energy expression and force field parameters.
- Introduction and simple molecular mechanics and molecular dynamics computations using force fields. Basic introduction to AMBER, GROMACS and LAMMPS

Wave Function and Density Functional Theory Based Methods

- Variational theorem. Review of HF-theory, electron correlation and introduction to Post-HF methods.
- Basis sets, Slater orbitals, Gaussian orbitals and contraction.

- Geometry optimization, calculation of thermodynamic parameters, vibrational frequencies and intensities, NMR and ESR parameters using elementary examples and a few representative molecules using Gaussian 16.

Density Functional Theory:

- A formal definition of electron density, Thomas-Fermi Model.
- Hohenberg-Kohn theorem, Kohn-Sham method, Fermi and Coulomb Holes. Introduction to local density and X-α method, Quest for approximate exchange-correlation functional.
- LDA-GGA-Meta GGA-Hybrid DFT and their implementation in Gaussian using a few sample molecules.

References

1. Understanding Molecular Simulations, D. Frenkel and B. Smit, second edition, Elsevier, 2001.
2. Computer Simulation of Liquids, M. P. Allen and D. J. Tildesley, second edition, Oxford University Press, 2017.
3. Exploring Chemistry with Electronic Structure Methods, J. B. Foresman and Aeleen Frisch, Gaussian Inc., 2015
4. A Chemists' Guide to Density Functional Theory, W. Koch & M. C. Holthausen, Wiley-VCH, 2001.
5. Introduction to Computational Chemistry, Frank Jensen, third edition, Wiley, 2017.
6. Modern Quantum chemistry, A. Szabo & N. S. Ostlund, McGraw-Hill, 1961 edition reprinted by Dover Publications, 1989.

CY6129: Advanced Methods in Experimental Physical Chemistry

Course Objective: To introduce the student to a number of state−of−the−art advanced research methods in physical chemistry, with regard to both the theoretical foundations and the experimental methods that are necessary to pursue modern experimental research in physical chemistry.

Course Outcomes:

Students should be able to:

Understand and Explain state−of−the−art advanced research methods in physical chemistry
Use and interpret experimental data from sophisticated equipment used in physical chemistry research

Thermal Properties of Chemical Systems: Principle, experimental measurement technique and applications of Differential scanning calorimetry (DSC), Differential thermal analysis (DTA), Thermomechanical analysis (TMA), Thermogravimetric analysis (TGA) and Simultaneous thermal analysis - STA (TGA/DSC). *Thermal conductivity:* Heat flow meter, Guarded hot plate method, Laser Flash (LFA) and Xenon Flash (XFA) techniques for thermal conductivity and thermal diffusivity measurements.

Transport Properties: *Viscosity*, glass capillary viscometer, rolling-ball viscometer and rotational viscometer; *Rheology*, Rheometers to characterize the rheological properties of materials, fluids, melts and solutions.

Electrochemical Methods: Voltammetry of reversible systems (Cyclic Voltammetry and Rotating Disk Voltammetry, Effect of Mass Transport); Mechanism of Electrode Processes (Steady-state Voltammetry, Chronoamperometry, and Chronopotentiometry); Electron-transfer kinetics (Current-overpotential curves, electron-transfer rates from voltammetry, Faradaic impedence).
X-ray diffraction and Rietveld analysis (Phase identification by X-ray diffraction, determination of crystal structure, quantitative phase analysis and small angle scattering). Scattering Methods, Particle Size Analysis (light scattering, intrinsic viscosity, x-ray and neutron scattering), gel permeation chromatography and relationship with particle size; zeta potential.

Examination of morphology of condensed phase using advanced microscopy (Kelvin Probe Microscopy, Environmental SEM, Cryo-TEM, Energy Dispersive X-ray Analysis).

Fluorescence spectroscopy, steady-state and time resolved spectroscopy, fluorescence and confocal imaging. Cavity ring-down spectroscopy, Applications of excimer lasers: reaction dynamics, photodissociation processes, and energies of dissociation; Transition State Spectroscopy and Femtosecond Chemistry, Time−integrated observation of Transition States of chemical reactions, Fast and Ultra−fast laser spectroscopy, Time−resolved spectroscopic observation of

Transition States. Techniques in kinetics of radical reactions in gas phase such as Laser induced fluorescence method.

Experimental Data Analysis, Correlation and Predictive Tools. Inspecting, cleansing, transforming, and modeling the experimental data, data integration. Empirical and semi-empirical formulas, correlations, group contribution methods and computational models for the prediction of experimental data.

Any three out of the six methods/modules (thermal, transport, electrochemical, x-ray diffraction, morphology, spectroscopy) shall be taught along with experimental data analysis-prediction of experimental data.

Suggested Reading Materials: Relevant Chapters from the following Books

Experiments in physical chemistry. Joseph W. Nibler, Carl W. Garland, Keith J. Stine, Judy E. Kim, McGraw-Hill Education, Boston, 2014.

Introduction to Thermal Analysis: Techniques and applications. Michael E. Brown, Springer Netherlands, 2001.

Principles and Applications of Thermal Analysis. Paul Gabbott, John Wiley & Sons, 2008.

Electrochemistry, 2nd Edition (Reprint 2010) by Philip H. Rieger, Chapman and Hall.

Elements of X-ray Diffraction, 3rd Edition. B. D. Cullity and S. R. Stock, Pearson, 2001.

Scanning and Transmission Electron Microscopy: An Introduction. Stanley L. Flegler, John W. Heckman, Karen L . Klomparens, Oxford University Press, 1993.

Methods in Physical Chemistry. Rolf Schaffer and Peter C. Schmidt. Wiley-VCH, 2012.

Fundamentals of Analytical Chemistry. Douglas A. Skoog, Donald M. West, F. James Holler, Stanley R. Crouch, Cengage Learning, Edition 9, 2013.

Principles of Fluorescence Spectroscopy, J R Lakowicz, Springer, Edition 3, 2006.

Laser Spectroscopy. Basic concepts and Instrumentation. W. Demtroder. **Third** edition **2004**, Springer international edition.

Assessment and Evaluation

All courses will have two sessional assessments, followed by an end semester examination. A minimum of 40% marks should be given to the sessional assessments and the remaining marks should be given for the end semester examination. The end semester examination will be of 3 hours duration.

In addition to several formative assessment techniques teachers use in the class room to assess the learning, the usual process for all the courses offered in the MSc program follow two sessional assessment tests, generally referred to as Quiz I and Quiz II, followed by a test called End Sem Examination.

The dates for all examinations will be announced by Department of Chemistry, IIT Madras in advance. Quiz and examination days are instruction free so as to enable students to focus on the exam preparation.

The marks/grades for all courses will be discussed in a common platform called ‘class committee’. A description of the working of class committee is given in the next page.

Class Committee and Students Feedback

Class committee is an academic body comprised of teachers and student representatives. There will be separate class committee meetings for I year MSc courses and II year MSc courses. Student representatives from the MSc batch for the class committee will be selected in the beginning of the first semester.

Class committee will meet minimum three times during the semester: in the beginning of the semester, after the quiz examinations and after the end semester examination.

The marks/grades of students will be displayed/discussed during the meetings and class committee chairperson request the concerned teacher to comment on student's performance, class conduct etc. The student representatives will provide feedback on the course conduct during the discussion and suggest ways to improve the learning environment.

Student feedback on course conduct plays a very important role in the class committee meetings. The student representatives should collect the feedback from all the students in the class regarding the conduct of each course and provide the information during the class committee meetings. A collective discussion will be facilitated by the class committee chairperson to identify solutions to address the teaching-learning issues.

Opportunity for Doing Ph D @ IIT Madras

Upgrading M. Sc. to Ph. D. Program

Interested to join for a Ph. D. program in the number one engineering Institute in the country?

The steps:

1. Qualifying CGPA is 8.00
2. CGPA will be computed at the end of 3rd semester and upgradation request can be given by M. Sc. students after 3rd semester.
3. The upgradation will be for M. Sc and Ph. D. Dual degree.
4. The M. Sc. students have to complete all the M. Sc courses as per M. Sc Curriculum and course requirement as per Ph. D. regulation and one/two special departmental courses XX6999 and XX7999 (XX stands for department code)of in lieu of M. Sc. project.
5. Comprehensive Viva Voce to be completed within three semesters after up-gradation.
6. Exit option will be considered after 6th semester.
7. Students can exercise exit option (with M.Sc degree alone) after 6th semester and have to meet the M. Sc. credit requirement of the respective departments.
8. M. Sc. degree will be awarded on successful submission on Ph. D. synopsis
9. The date of award of M. Sc. degree in the M. Sc. certificate shall be printed as date of completion of M. Sc. course requirements for which, certificate of date of completion of M. Sc. courses to be issued by the respective HoDs.
10. Other requirements for Ph. D. such as seminar, research proposal meeting, defense etc remains the same as per Ph. D. regulations.

Contact Details

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*Contact CY office to know the names of the faculty advisors for the current academic year