Master of Science Program in Chemistry

July 2015

Indian Institute of Technology Jodhpur

Master of Science (M.Sc.) Program in Chemistry

Curriculum

Cat.	Course Number, Course Title	L-T-P	Credits		Cat.	Course Number, Course Title	L-T-P	Credits
I Semester					**II Semester**			
C	CY 511 Reactions and Mechanisms	3-0-3	4		C	CY 521 Physical Organic Chemistry	3-0-0	3
C	CY 512 Transition Metal Chemistry	3-0-0	3		C	CY 522 Main Group Chemistry	3-0-3	4
C	CY 513 Statistical Thermodynamics and Chemical Kinetics	3-0-3	4		C	CY 523 Solid State and Material Chemistry	3-0-0	3
C	CY 514 Quantum Chemistry and Spectroscopy	3-0-0	3		C	CY 524 Chemical Binding	3-0-3	4
C	CY 515 Mathematical and Numerical Techniques for Chemists	3-0-0	3		C	CY 525 Organometallic and Bio-Inorganic Chemistry	3-0-0	3
		Total	**17**				*Total*	**17**
III Semester					**IV Semester**			
C	CY 612 Organic Synthesis	3-0-0	3		E	CY 613 Analytical and Spectroscopic Techniques	3-0-0	3
R	Thesis		15		R	Thesis		15
		Total	**18**				*Total*	**18**

Electives

CY751	Quantum Computing	CY759	Advance Material Design
CY752	Principles of Nuclear Magnetic Resonance	CY760	Polymer Dynamics
CY753	Analytical Techniques and Spectroscopy	CY761	Art in Organic Synthesis
CY754	Statistical Mechanics and Molecular Simulations	CY762	Quantum Chemistry
CY755	Advance Catalysis	CY763	Catalysis for Energy
CY756	Group Theory and Molecular Spectroscopy	CY764	Chemical Reaction Dynamics
CY757	Chemical Binding	CY765	Molecular Dynamics Simulations
CY758	Stochastic Problems in Biophysics	CY766	Stereochemistry of Organic Compounds
		CY768	Water Chemistry
		CY769	Sustainable catalytic Design

S. No.	Category	Course Category Title	Total Courses	Total Credits
1	C	*Compulsory*	12	40
2	R	*Thesis*	1	30
		Total	**11**	**70**

Course Title	**Organic Reactions and Mechanisms**	Course No.	**CY 511**
Department	Chemistry	Structure (L-T-P:C)	3 0 3 4
Offered for	M.Sc. (Chemistry) Students	Status	Compulsory
Pre-requisite	*Consent of Teacher*		

Objectives

The objectives of this course are to

1. Give students a better insight into the methods by which organic reaction mechanisms are studied, and
2. Broaden their knowledge of reaction mechanisms in ionic and radical system.

Learning Outcomes

Students will be able to

1. Draw mechanisms for complex reactions, to predict reactivity, to appreciate how orbital interactions affect structure and reactivity; and
2. Propose more complex syntheses than previously.

Contents

1. **Organic synthesis**: Principle of Stereochemistry, conformational analysis,isomerization and chirality, reactive intermediate and Organic Reaction mechanism, aromaticity, name reactions, transformation and rearrangement, principle and application of organic photochemistry, nuclephilic, electrophilic and free redical reaction, chemoselectivity, regeioselctivity, enantioselectivity, protectecting group. Hetrocyclic Chemistry
2. **Introduction:** Reaction mechanism and its need, Concerted vs. stepwise processes; transition states and intermediates; molecularity. Early and late transition states; the Hammond postulate. Rate equations and their integrated forms; measuring rates and rate constants
3. **Acids and bases**: The pKa scale and its meaning; pKas of common acids; when to draw protons in a mechanism - and when not to; specific and general acid and base catalysis. Acid and base-mediated hydrolysis of esters; classification of different mechanisms
4. **Rearrangements and migrations**: Cationic rearrangements; Baeyer-Villiger and Beckmann rearrangements; migratory aptitudes.
5. **Crossover experiments**: The basis of crossover experiments; examples in the Fries and Claisen rearrangements; ozonolysis.
6. **Electronic Effects on Reaction Mechanisms**: Electronic effects; linear free energy relationships; Hammett plots; the significance of σ, σ^+ and ρ and Isotopic labelling.

Organic Chemistry Laboratory

1. Extraction: Separation of an Acidic, a Basic and a Neutral Substance
2. Thin Layer Chromatography (TLC): extraction of Spinach Pigments
3. Column Chromatography: Food color and pigment separation
4. Dehydration of Methylcyclohexanols: Prepration of methylcyclohexene
5. The Diels-Alder Reaction of a Conjugated Diene in Eucalyptus Oil
6. The Friedel-Crafts Acylation of Ferrocene

7. Reduction and Oxidation of Organic Compounds
8. Identification of an Aldehyde and Ketone
9. Green Chemistry: A Solvent-Free Aldol Condensation

References

1. Sykes, P. (2013) *A Guidebook to Mechanism in Organic Chemistry*, Longman,
2. Gossman, R.B. (2008) *The Art of Writing Reasonable Organic Reaction Mechanism*, Springer,
3. McMurry (2013) *Organic Chemistry*, 8th Ed., Cengage
4. NPTEL Lecturers : http://nptel.ac.in/courses/104101005/
5. Vogel, A. I. (2012) *Textbook of Practical Organic Chemistry*
6. Prichard, E. (1995) *Quality in Analytical Chemistry Laboratory*
7. Ault, A. (1998) *Techniques and Experiments for Organic Chemistry*

Course Title	**Transition Metal Chemistry**	Course No.	**CY 512**
Department	Chemistry	Structure (L-T-P:C)	3 0 0 3
Offered for	M.Sc. (Chemistry) Students	Status	Compulsory
Pre-requisite	*Consent of Teacher*		

Objectives

1. The objectives of this course are provides student with an overview of transition metal chemistry which forms a foundation for students pursuing further studies in chemistry.

Learning Outcomes

1. Explain the bonding characteristics in coordination compounds in term of Crystal Field Theory and Molecular Orbital Theory.
2. Physical properties and reactivities of selected transition metal complexes with their structure and bonding.
3. Development of logical and critical thinking about transition metal chemistry.

Contents

1. *Coordination Compounds:* Structure and Bonding
2. *Crystal Field Theory:* Introduction to VBT and MOT, The basics of Crystal Field Theory, Crystal Field Stabilisation Energies, origin and effects on structures and thermodynamic properties. High and low spin complex, pairing energy, John-Teller theorem , Irving Williams series
3. *Spectroscopic properties transition metal complexes:* Color of the complexes, Selection rules for electronic transitions. Splitting of the free ion energy levels in Octahedral and Tetrahedral complexes. Term Symbol, Orgel, and Tanabe-Sugano diagrams, Spectra of aquated metal ions. The spectra of octahedral and tetrahedral complexes, Factors affecting positions, intensities and shapes of absorption bands.
4. *Magnetic Susceptibilities of transition metal complexes:* Effect of orbital contributions arising from ground and excited states, Deviation from the spin-only approximation, Experimental determination of magnetic moments, Interpretation of data. Ferromagnetic and antiferromagnetic properties.

References

1. NPTEL Lectures http://nptel.ac.in/courses/104105033/
2. Cotton, F. A., Wilkinson, G., Murillo, C. A., and Bochmann, M., (2010) *Basic Inorganic Chemistry*, John Wiley & Sons, New York
3. Kettle, S. F. A., (2010) *Physical Inorganic Chemistry: A Coordination Chemistry Approach*, Springer
4. Astruc, D., (2013) *Organometallic Chemistry and Catalysis*, Springer
5. Crabtree, R. H., (2009) *The Organometallic Chemistry of Transition Metals*, John Wiley & Sons, New York

Course Title	**Chemical Kinetics and Statistical Thermodynamics**	Course No.	***CY513***			
	Chemistry	Structure (LTPC)	3	0	0	3
Offered for	M. Sc.	Status	Core		Elective	

Objectives

1. To understand the inter-relationships of thermodynamics and statistical mechanics
2. To understand the bridge between statistical mechanics and kinetics

Learning Outcomes

1. Ability to predict properties of many-body systems starting from its microscopic constituents and their interactions
2. Ability to translate complex phenomena into simple models and develop approaches for solving these models

Course Content

1. Thermodynamic functions and standard states, Criteria for equilibrium and spontaneity, Maxwell's relations and Nernst equation.
2. Introduction to Statistical Methods, Micro and Macro states, Ensemble theory (micro-canonical, canonical, isobaric, grand-canonical).
3. Random walk, Probability distribution, Central Limit theorem, Partition functions, Distribution functions.
4. Ion-ion distribution function, Debye-Huckel theory, activity coefficient.
5. Rate Law and mechanism of chemical reactions, thermodynamical relations, influence of solvent properties on rates.
6. Theory of reaction rates, transition state theory, activation energy, relation with thermodynamics, unimolecular and bimolecular reactions, Lindemann, Hinshelwood theory, potential energy surfaces.
7. Electrode kinetics, Butler-Volmer equation, polarizable and non-polarizable electrodes.

Physical Chemistry Laboratory

1. Determination of enthalpy of fusion by freezing point depression and calculation of heat capacities of metal – Application of differential scanning calorimeter.
2. Thermogravimetric analysis of polystyrene beads.
3. Cyclic voltammetry experiments.
4. Fluorescence and kinetic analysis of amount of vitamin in vitamin pills.
5. Determination of surface coverage of an adsorbate on silica by FTIR.
6. Powder XRD analysis of a hydrogen storage material.
7. Formation of Micelle – experiment on surface tension.
8. Experiment on electrode kinetics – hydrogen evolution.
9. Determination of PI of amino acid using potentiometer.
10. Study of phase equilibrium.

References

1. Frederick, R. (2010) *Fundamental of Statistical and Thermal Physics*, McGraw-Hill, New York
2. Donald, A. M., (2000) *Statistical Mechanics*, University Science books

3. Laidler K. J. (2009) *Chemical Kinetics*, 3rd Ed. Pearson
4. Albery W. J. (1975) *Electrode Kinetics*, Clarendon Press, Oxford
5. Steinfeld, J. I., Francisco, J. S. and Hase, W. L. (1998) *Chemical Kinetics and Dynamics*, Prentice Hall
6. Bockris J. O'M. and Reddy A. K. N. (1998) *Modern Electrochemistry, Vol 1 and 2*, Plenum Press
7. Halpern, A. M., McBane, G. C., (2006) *Experimental Physical Chemistry: A Laboratory Text Book*, 3rd Ed., W. H. Freeman

Course Title	**Quantum Chemistry and Spectroscopy**	Course No.	**CY 514**
Department	Chemistry	Structure (L-T-P:C)	3 0 0 3
Offered for	M.Sc. (Chemistry) Students	Status	Compulsory
Pre-requisite	Basic Physical Chemistry		

Objectives

1. The course is an attempt to provide an advanced level understanding of quantum chemistry
2. A few applications of quantum mechanics to chemistry will be shown
3. Relation between fundamentals of spectroscopy and quantum chemistry will be established

Learning Outcomes

1. Understanding of quantum mechanics and applications to chemistry problems such as minimum energy path search, single point calculation and geometry optimization.
2. Application of spectroscopic methods as analytical tool in chemistry, biology, material science, medicine

Contents

1. *Fundamentals:* Old Quantum theory, Correspondence principle, Bohr-Sommerfeld quantization, Wave-particle duality, Stern-Gerlach experiment
2. *Mathematical Formalism:* Operators, Eigenfunctions and eigenvalues, Operators in quantum mechanics, expectation values
3. *Exactly Solvable Problems:* Time independent and time dependent wave equation, Particle confined to infinite and finite potential wells, Harmonic oscillator, Rigid rotor, Hydrogen atom
4. *Approximation Methods:* Variational principle, Perturbation theory, Energy and wavefunction corrections
5. *Many electron atoms and molecules:* Born-Oppenheimer approximation, Hartree-Fock self-consistent field method, Electron correlation Spin-orbit interaction, Density Functional theory
6. *Introduction to spectroscopy:* Introduction to rotational, vibrational spectroscopy, and NMR spectroscopy, electronic transitions, Frank-Condon principles, vertical transitions – selection rules, parity, symmetry and spin selection rule, - Jablonski diagram and Beer-Lambert law

References

1. Levine, I. N. (1983) *Quantum Chemistry*, Allyn and Bacon
2. McQuarrie, D. A. (1983) *Quantum Mechanics*, University Science Books
3. Bernath, P. F. (2005) *Spectra of Atoms and Molecules*, 2nd Ed., Oxford University Press
4. Banwell, C. N., (2010) *Fundamentals of Molecular Spectroscopy*, Tata McGraw Hill

Course Title	***Mathematics and Numerical Techniques for Chemists***	Course No.	**CY515**
Department	Chemistry	Structure	3 0 0 3
Offered for	M.Sc. (Chemistry) Students	Status	Compulsory
Pre-requisite	*Basic Quantum Mechanics*		

Objectives
1. Basic mathematics and numerical techniques required for Chemistry students
2. Practical knowledge on error analysis to be used in chemistry laboratory

Learning Outcomes
1. Ability to analyze data and perform error analyze on the chemistry laboratory data.
2. Ability to understand and appreciate the mathematics behind chemical theories

Course Content
1. *Ordinary and Partial Differential Equations and Special Functions*
2. *Fourier and Laplace Transforms*
3. *Matrix Methods:* Orthogonal and Unitary Matrices, Diagonalization, Eigenvalues and Eigenvectors
4. Group theory and representations of Symmetry operations by Matrices, Character Tables
5. *Numerical Methods:* Errors in Data, Distribution of Errors, Central Limit Theorem
6. Power Series and Conversions, Interpolation and Curve Fitting, Roots of Equations, Algorithms for Matrix, Inversion and Diagonalization
7. *Use of Matlab and Scilab for Numerical Methods*

References

1. Kreyszig, E., (2011) *Advanced Engineering Mathematics*, 9th Ed., Wiley
2. Cotton, F. A., (2008) *Chemical Applications of Group Theory*, 3rd Ed., Wiley India
3. Louis, L., (1991) *A Practical Guide to Data Analysis for Physical Science students*, Cambridge University Press
4. Louis, L., (2005) *Mathematics for Science Students*, Cambridge University Press
5. Arfken, W. and Harris, P. (2012) *Mathematical Methods for Physicists*, 7th ed., Elsevier

Course Title	**Physical Organic Chemistry**	Course No	**CY 521**
Department	Chemistry	Structure (L-T-P:C)	3 0 0 3
Offered for	M.Sc. (Chemistry) Students	Status	Compulsory
Pre-requisite	Basic Physical and Organic Chemistry		

Objectives

1. To provide physical concepts of organic chemistry
2. To make connections between organic and physical chemistry

Learning Outcome

The Students are expected to be able to apply the fundamentals towards understanding the mechanism of a reaction, modeling of organic reactions.

Contents

1. *Introduction:* Conceptual Organic Chemistry: Review of basic concepts of inductive effect, electromeric effect, resonance effect, hyperconjugation, the formalism of curved arrow mechanisms.
2. *Stereoelectronic Effects in Organic Chemistry:* Orbital Symmetry and Frontier Orbitals, Participation of sigma and pi bonds, Quantitative aspects of stereochemistry, Conformational analysis of organic and biomolecules, Evaluation of aromaticity by spectral methods (UV, NMR), Antiaromaticity.
3. *Chemical Equilibria and Chemical Reactivity:* Reactive Intermediates, Concerted reactions, examples of solvent effect from SN2 substitution and E2 elimination reaction - introduction to carbon acids, pKa of weak acids.
4. *Chemical Kinetics:* Captodative Effect, interpretation of Kinetic Data, isotope Effects, Hammond's Postulate, Thermodynamic and Kinetic Control, Kinetics of chain reactions
5. *Concerted Reaction:* Pericyclic Reactions and Photochemistry.

References

1. NPTEL Lectures http://nptel.ac.in/syllabus/104106030/
2. Koswer, E.M. (2009) *An Introduction to Physical Organic Chemistry* (International Ed.), John Wiley
3. March, J. (2013) *Advanced Organic Chemistry*, 7th ed., McGraw Hill, New York
4. Lowry, T. H., and Richardson, K. S., (2010) *Mechanism and Theory in Organic Chemistry*, Harper and Row

Course Title	**Main Group Chemistry**	Course No	**CY 522**
Department	Chemistry	Structure (L-T-P:C)	3 0 3 4
Offered for	M.Sc. (Chemistry) Students	Status	Compulsory
Pre-requisite	Basic Physical and Organic Chemistry		

Objectives

To give better insight into main group chemistry elements as well as to broaden their knowledge of about the properties and behavior of Main Group elements

Learning Outcome

1. Appreciate trends in chemical and physical behavior of main group metal compounds and how they may be controlled (tuned) by particular types of ligand
2. Combine spectroscopic, structural and other experimental data to determine identities of p-block coordination compounds and to rationalize their properties
3. Appreciate some important and emerging applications of main group complexes and materials and the key features necessary for these

Contents

1. *Chemistry of main group elements:* Borons, silicon, phosphorous compounds, boranes, silanes, phospholanes, borazines, BN, SiN,P-N,S-N rings synthesis, structure and bonding. Hydrides, halides, oxides, oxiacids, nitrides, and allotropes of Carbon. Chemistry of Nobel gases, pseudo halogen and inner halogen compounds and acid-base concept.
2. *Applications of main group metals:* An overview of the range of applications of main group complexes, and materials derived from them- Frustrated Lewis pairs small molecule activation - Synthetic uses of main group complexes. Oxidizing/reducing agents - Precursors for materials deposition. Deposition of thin films of materials, with a strong focus on Chemical Vapour Deposition (CVD)- Uses of thin films (TCO, diamond, other semiconductors etc.) - CVD vs other deposition techniques (ALD, sol-gel, electrodeposition) - Vaporization techniques (AA, LP, AP, SCF etc.) - Principles of precursor design- Post-deposition characterization techniques
3. Overview of the development of radio-labelled p-block complexes for applications in PET and SPECT imaging

Inorganic Chemistry Laboratory

1. Non-metal complex: Synthesis and characterization of bispyridine iodide nitrate
2. Solid phase synthesis of *trans*-bis glycinato copper(II) and characterization
3. Synthesis of penta amminechlorocobalt(III)chloride and its spectroscopic properties
4. Influence of ligand field tetragonality on the ground state spin of nickel(ii) complexes with NH3 and H2O and ethylene diamine.
5. Preparation and magnetic properties of Fe^{III}(acac) complex
6. Preparation of TiO_2 from Titanium Isopropoxide
7. Preparation, Characterization and water treatment application of Hydroxyapatite
8. Iodide oxidation with hydrogen peroxide

References

1. Greenwood, N.N. (2013) *Chemistry of the Elements*, Elsevier
2. Norman, N. C., (2009) *Periodicity and the p-Block Elements*, Oxford Primer Nos. 51, Oxford University Press
3. Housecroft, C. E., and Sharpe, A. G., (2008) *Inorganic Chemistry*, 3rd Ed., Pearson
4. NPTEL Lectures: http://nptel.ac.in/courses/104101006/

Course Title	**Solid State and Material Chemistry**	Course No.	**CY 523**
Department	Chemistry	Structure (L-T-P:C)	3 0 0 3
Offered for	M.Sc. (Chemistry) Students	Status	Compulsory
Pre-requisite	Basic Physical Chemistry		

Objectives

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

Learning Outcomes

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

Contents

1. *Structure of Solids:* Crystalline and Amorphous, diffraction techniques, symmetry and point groups, packing in solids, classification, lattice energy, bonding, structures: NaCl, TiO_2, ZnS, wurtzite, perovskite, covalent and ionic solids.
2. *Crystal defects:* nonstoichiometry, cluster, diffusion, Fick's Law and Kirkenall effect.
3. *Solid state reaction:* Methods of preparation, reactivity of solids, decomposition mechanism, single crystal growth and thin film deposition.
4. *Band theory:* Intrinsic and extrinsic semiconductors, Hall effect, Thomson, Peltier and Seebeck effects, insulators
5. *Properties of Solids:* Magnetic, Electrical and Optical properties, Different type of Magnetism and Super Conductivity, Colloids and Surface Phenomenon, soft and hard materials, Nanomaterials, Quantum Dots

References

1. NPTEL Courses http://nptel.ac.in/courses/104103019/2
2. NPTEL Lectures http://nptel.ac.in/courses/104103019/7
3. West, A.R. (2015) *Solid State Chemistry and Its Applications*, John Wiley & Sons
4. Kittel, C. (2010) *Introduction to Solid State Physics*, 6^{th} Ed., Wiley
5. Cheetham, A. K. and Day, P. (1997) *Solid State Chemistry Compounds*, Clarendon Press, Oxford

Course Title	***Chemical Binding***	Course No.	**CY524**
Department	Chemistry	Structure	3 0 3 4
Offered for	M.Sc. (Chemistry) Students	Status	Compulsory
Pre-requisite	*Basic Quantum Mechanics*		

Objectives

1. High level understanding of a chemical bond using quantum mechanics.
2. Knowledge of modern techniques in quantum chemistry

Learning Outcomes

Ability to use modern quantum chemistry techniques to solve problems and theoretical understanding of a chemical bond

Content

1. *Electronic structure:* Many electron atoms, Variational principle, Born-Oppenheimer approximation, H2+ ion, homo and hetero nuclear diatomic molecules, Valence bond and Molecular orbital theories.
2. *Hartree-Fock (HF) and post HF theories:* HF theory of atoms and molecules, Self-consistent field wavefunction, configuration interaction wavefunction, Moller-Plesset perturbation theory and CI calculations
3. *Semi-empirical methods:* Introduction to CNDO (Complete neglect of differential overlap), INDO (Intermediate neglect of differential overlap) and NDDO (Neglect of of diatomic differential overlap)
4. *Density functional theory (DFT):* Principles of DFT, Commercial Functionals Time dependent perturbation theory, Transition probability and Reaction cross section Intermolecular forces and their determination. Use of Gaussian and other public domain softwares to perform simple electronic structure calculations

References

1. Levine, I. N. (2000) *Quantum Chemistry*, Pearson
2. Lowe, J. P., *Elementary Quantum Chemistry*, Academic Press
3. Szabo, A. and Ostlund, N. S. (1996) *Modern Quantum Chemistry*, Dover

Course Title	**Organometallic and Bio-Inorganic Chemistry**	Course No.	**CY 525**
Department	Chemistry	Structure (L-T-P:C)	3 0 0 3
Offered for	M.Sc. (Chemistry) Students	Status	Compulsory
Pre-requisite	Basic Physical Chemistry		

Objectives

1. To learn about the goals and methods of chemists that aim to mimic biological systems.
2. To learn about selected organometallic and inorganic complexes that do a good job of mimicking biological catalysis.
3. To describe the synthesis and general properties of organometallic compounds
4. An introductory understanding of Bio-inorganic chemistry

Learning Outcomes

1. To recognize organometallic ligands and compounds
2. Knowledge of fundamental organometallic reactions
3. Knowledge of a variety of or oganometallic based catalytic
4. reactions, including a mechanistic understanding including enzymatic reactions

Contents

1. *Structure, bonding and properties of organometallic compounds:* Ligands (carbonyl, olefins, phosphine, hydride, alkyls, carbines, carbenes). Compounds with carbonyl, olefins - effective atomic number (EAN) rule. Classification of ligands – sigma, pi-donor, pi-acceptor).
2. *Bonding in organometallics:* sigma and pi-back bonding. Synthesis of organometallic compounds. Characterization by FTIR.
3. *Organometallic Reaction:* Oxidative addition, reductive elimination, CO insertion and migration reactions. Applications of Organometallic compounds in homogeneous catalysis –hydrogenation reaction, hydroformylation, Monsanto acetic acid synthesis, C-C coupling reactions, and metathesis. Heterogeneous catalysis- Zeigler-Natta olefin polymerization.
4. *Role of metal-ions in biological systems:* O2 transport and storage - hemoglobin, myoglobin, hemerythrin, hemocynanin, chlorophyll and oxygen evolving complex. Electron transport proteins – blue copper proteins, cytochromes, Fe-S clusters. Oxygenation by cytochrome P450, vitamin B12, Cu-Zn-superoxide dismutase, hydrolases and peptidases, nitrogenase.

References

1. NPTEL Course http://nptel.ac.in/courses/104105031/; http://nptel.ac.in/courses/104108062/
2. Astruc, D. (2013) *Organometallic Chemistry and Catalysis*, Springer
3. Crabtree, R. H. (2009) *The organometallic chemistry of transition metals*, John Wiley & Sons, New York
4. Gray, H. B. (2006) *Biological Inorganic Chemistry: Structure and Reactivity*, University Science Books

Course Title	***Organic Synthesis***	Course No.	**CY 612**
Department	Chemistry	Structure	3 0 0 3
Offered for	M.Sc. (Chemistry) Students	Status	Compulsory
Pre-requisite			

Objectives

The objectives of this course are to

1. Knowledge of key aspects of retrosynthesis of complex organic molecules.
2. An understanding of the fundamental mechanistic aspect of chemical transformations

Learning Outcomes

1. An understanding of some total synthesis.
2. The basic knowledge, skills and experience on wise strategy and plan to design a molecule.

Course Content

1. *Introduction to Strategies for the Synthesis of Complex Molecules:* General principles of retrosynthetic analysis and general strategies for stereochemical control. Protecting and deporting groups, one pot synthesis.
2. *Application of carbaninon in organic synthesis:* Chemistry of "carbanionic" synthetic building blocks. Directed metalation for the generation of organolithium compounds, and discussion of alkenyl and alkynyl-metal compounds.
3. *Synthetic Application of organometallic species:* Electrophilic Substitution Reactions: Reaction of Caranion with alkyl halides, sulfonates, and related electrophilic substitution reactions. Stereocontrolled alkylation.
4. *Addition to C=O group:* Stereocontrol elements in 1,2-additions to carbonyl compounds. Stereocontrolled reduction of ketones and 1,2-addition of organometallic compounds to carbonyl groups.
5. *Addition of Allylmetal Compounds to unsaturated bond:* Introduction to reactions of carbocation with carbon-carbon pi bonds including organosilanes and stannanes.
6. *Functional Group Transformations:* Including reduction, oxidation, and functional group interconversions by nucleophilic substitution.
7. *Classic Synthesis:* Penicillin, Estron and Quinine

References

1. NPTEL Lecture http://www.nptel.ac.in/courses/104103022/
2. Jonathan C., Greeves, N. and Warren, S. (2010) *Organic Chemistry*, Oxford University
3. Nicolaou, K. C. and Sorensen, E. J. (2003). *Classics in Total Synthesis: Targets, Strategies and Methods*, 4th Ed., Wiley-VCH
4. Warren, S.; and Wyatt. P. (2008) *Organic Synthesis: The Disconnection Approach*, 3rd Ed., Wiley-VCH

Course Title	***Analytical and Spectroscopic Techniques***	Course No.	**CY623**
	Chemistry	Structure (LTPC)	3 0 0 3
Offered for	MSc., PhD	Status	Core √ *Elective*

Objectives

1. Introduction to a few spectroscopic methods used as analytical techniques in various fields of science and engineering.
2. Introduction to theoretical background of these methods along with their instrumentation and application.
3. Enable students to use such methods whenever needed by giving hands on experience with available instruments in the Institute.

Learning Outcomes

1. Basic understanding of the theoretical background of various spectroscopic techniques.
2. Application of spectroscopic methods as analytical tool in chemistry, biology, material science, medicine.
3. Exposure to various spectrometers available in the institute.

Course Content

1. *Introduction to Spectroscopy:* Properties of electromagnetic radiation – interaction of radiation with matter – classical picture – uncertainty and question of time scale – intensity of spectral line and line shape – Sensitivity and resolution of spectral line – Fourier Transformation
2. *UV-VIS and Fluorescence Spectroscopy:* Basic principle, Chromophores – Laws of photochemistry, Beer-Lambert law, electronic energy levels, Solvent relaxation, Jablonski diagram, Frank-Condon principle, Excited state life time, excited state kinetics, solvent effect, quantum yield expression and Stern-Volmer equation, excimer and exciplex, kinetics of luminescence quenching, photoinduced energy transfer, FRET. Instrumentation and applications
3. *Infrared and Raman Spectroscopy:* Basic principle; Organic functional group identification through IR spectroscopy, IR and Raman activity, Raman shift, Instrumentation and applications
4. *NMR Spectroscopy:* Basic principle, spin-1/2 nuclei and energy level diagram, Zeeman splitting, introduction to NMR parameters - chemical shift and spin-spin coupling, introduction to AB, AX, AMX spin system, 1D 1H and 13C NMR for structure elucidation, longitudinal and transverse relaxation processes, measurement of relaxation rates, NOE, 2D NMR, correlation spectroscopy -Instrumentation and application
5. *EPR Spectroscopy:* Basic principle, Zeeman splitting, g-values, hyperfine coupling, instrumentation and applications in inorganic compound with unpaired electrons.
6. *Mass Spectrometry:* Basic principle, ionization technique, molecular ion, fragmentation processes. Instrumentation and application

References

1. Farrar, T. C. and Becker, E.D. (1971) *Pulse and Fourier Transform NMR*, Academic Press, New York
2. Silverstein, R. M., Bassler, G. C., and Morril, T. C. (1991) *Spectroscopic Identification of*

Organic Compounds, Wiley
3. Gunther, H. (1995) *NMR Spectroscopy*, 2nd Ed., Wiley-VCH
4. Banwell, C. N., (2008) *Fundamentals of Molecular Spectroscopy*, Tata McGraw Hill
5. Bernath, P. F., (2005) *Spectra of Atoms and Molecules*, 2nd Ed., Oxford University Press
6. Lakowicz, J. R., (2006) *Principles of Fluorescence Spectroscopy*, 4th Ed., Springer, New York
7. Hagen, W. R., (2009) Biomolecular EPR, CRC Press, Taylor and Francis Group, 2009

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Course Booklet for M.Sc. (Chemistry)

2015