MSc Chemistry Curriculum Structure

Course Curriculum Structure (2019 onwards)

Cat.	*Course Number, Course Title*	*L-T-P-D*	*Credits*		*Cat.*	*Course Number, Course Title*	*L-T-P-D*	*Credits*
I Semester					**II Semester**			
C	CY5XX: Organic Reactions and Mechanisms	3-0-0-0	3		C	CY5XX Organic Synthesis	3-0-0-0	3
C	CY5XX:Transition Metal and Organometallic Chemistry	3-0-0-0	3		C	CY5XX Solid State and Material Chemistry	3-0-0-0	3
C	CY5XX: Quantum Chemistry and Spectroscopy	3-0-0-0	3		C	CY5XX: Molecular Thermodynamics and Chemical Kinetics	3-0-0-0	3
C	CY5XX: Physical Organic Chemistry	3-0-0-0	3		C	CY5XX: Theory and Applications of spectroscopic techniques	3-0-0-0	3
C	CY5XX: Main Group and Bioinorganic Chemistry	3-0-0-0	3		E	Program elective-1	3-0-0-0	3
C	Lab-1:Organic Laboratory	0-0-3-0	1.5		C	Lab-3: Physical Laboratory	0-0-3-0	1.5
C	Lab-2: Inorganic Chemistry Laboratory	0-0-3-0	1.5		C	Minor Project	0-0-3-0	1.5
C	Hands on -1	0-0-3-0	1.5		C	Hands on-2	0-0-3-0	1.5
	Total		**19.5**			*Total*		**19.5**

III Semester					**IV Semester**			
E	Open elective-1	3-0-0-0	3		E	Program Elective-5	3-0-0-0	3
E	Program Elective-2	3-0-0-0	3		E	Program Elective-6	3-0-0-0	3
E	Program Elective-3	0-0-3-0	3		E	Open Elective -2	3-0-0-0	3
E	Program Elective-4	3-0-0-0	3		R	Project	0-0-0-10	10
C	Lab-4:Computational Lab	0-0-1-0	1.5					
R	Project	0-0-0-5	5					
C	Seminar	0-0-1-0	0.5					
	Total		**19**			*Total*		**19**
** Open Elective Courses can be taken in the third semester as well*								

Total Credits: 77

Contents

Core Courses

Title	**Organic Reactions and Mechanisms**	Number	CY5XX
Department	Chemistry	L-T-P [C]	3-0-0 [3]
Offered for	M.Sc. (CY) Program	Type	Compulsory
Prerequisite	Prior consent of the instructor		

Objectives

The instructor will:

1. To give students a better insight into the mechanism of diverse set of organic reactions
2. To broaden their knowledge in fundamental organic chemistry with regard to efficiency and selectivity of organic reactions.

Learning Outcomes

The students are expected to:

1. The students are expected to be able to draw mechanisms for complex reactions
2. Understand and predict the orbital interactions involved in organic reactions

Contents

Introduction: reaction mechanism and its need, methods of determination of reaction mechanism, concerted versus stepwise processes, transition states and intermediates, early and late transition states, crossover experiments and examples, molecular orbital interaction of common functional groups (7 lectures)
Acids and bases: the pKa scale and its interpretation, pKa's of common acids; specific and general acid and base catalysis (3 lectures)
Classification of reactions: introduction to substitution, elimination and addition reactions, aromaticity and aromatic substitution reactions (9 lectures)
Stereochemistry: basics of Stereochemistry, stereochemistry of aliphatic compounds, conformational analysis of acyclic and cyclic compounds, (6 lectures)
Selectivity: chemoselectivity, regioseIctivity, and stereoselectivity (4 lectures)
Radical Chemistry: Basics of radicals, radical initiators, radical halogenation of alkanes, radical name reactions (6 lectures)
Rearrangements and migrations: cationic rearrangements, carbanionic rearrangements, carbene/carbenoid based rearrangements (7 lectures)

Textbooks

1. Sykes,P., (2013), *A Guidebook to Mechanism in Organic Chemistry*, 6th Edition, Longman
2. Clayden,J., Greeves,N., and Warren,S., (2012), *Organic Chemistry*, 2nd Edition, Oxford
3. Carey,F.A., and Sundberg,R.J., (2007) *Advanced Organic Chemistry, Part A: Structure and Mechanisms*, 4th Edition, Plenum

Reference Books

1. Gossman,R.B., (2008), *The Art of Writing Reasonable Organic Reaction Mechanism*, Springer

Preparatory Course Material

1.Sunoj,R.B., *Organic Reaction Mechanism*, NPTEL Course Material, Department of Chemistry, Indian Institute of Technology Bombay, http://nptel.ac.in/courses/104101005/

Title	**Physical Organic Chemistry**	Number	CY5XX
Department	Chemistry	L-T-P [C]	3-0-0 [3]
Offered for	M.Sc. (CY) Program	Type	Compulsory
Prerequisite			

Objectives

The instructor will:

1. To provide physical concepts of organic chemistry
2. To provide knowledge in pericyclic and photochemical reactions

Learning Outcomes

The students are expected to:

1. Be able to understand the course of organic reactions with regard to physical concepts and stereochemical models
2. Develop an in-depth knowledge with mechanistic understanding in pericyclic and photochemical reactions and apply those in the synthesis of organic compounds

Contents

Introduction: Brief review of basic concepts of inductive effect, Electromeric effect, Resonance effect, Hyperconjugation, Captodative Effect (4 lectures)
Stereoelectronic Effects: Participation of sigma and pi bonds in transition state, Orbital symmetry and frontier orbitals, , Hammond's Postulate, Hammette Plot, Curtin–Hammett principle (6 lectures)
Stereochemical Models: Cram Model, Felkin-Anh Model, Chelation Model, Zimmerman-Traxler Model (7 lectures)
Pericyclic Reactions: Introduction of pericyclic reactions, Classifications, Cycloaddition, Electrocyclic, Sigmatropic, Group transfer reactions (15 lectures)
Photochemistry: Basic principles of photochemistry, Photochemical reaction of cyclic and acyclic carbonyl compounds including enones and dienones, photochemistry of alkenes, dienes, aromatic compounds (10 lectures)

Textbooks

1. Anslyn, E. V. and Dougherty, D. A., (2006),Modern Physical Organic Chemistry, University Science Books
2. Singh, J. and Singh, J., (2012), Photochemistry and Pericyclic Reactions, 3rd Edition. New Age

Reference Books

1. Smith, M. B., (2016), March's *Advanced Organic Chemistry*, 7th Edition. Wiley
2. Koswer, E.M., (2009), *An Introduction to Physical Organic Chemistry,* International Edition. Wiley
3. Carey, F. A. and Sundberg, R. J., (2007), *Advanced Organic Chemistry Part A: Structure and Mechanisms*, 5th Edition. Springer
4. Carey, F. A. and Sundberg, R. J. (2007), *Advanced Organic Chemistry Part B: Reactions and Synthesis*, 5th Edition. Springer

Preparatory Course Material

1. Singh, N.D. P., *Organic Chemistry and Pericyclic Reactions*, NPTEL Course material, Department of Chemistry, Indian Institute of Technology Kharagpur, http://www.nptel.ac.in/courses/ 104105071/

Title	**Organic Synthesis**	Number	CY5XX
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	M.Sc. (CY) Program	Type	Compulsory
Prerequisite			

Objectives

The instructor will:

1. To provide an understanding of diverse chemical reactions and their application in synthesis
2. To provide knowledge of key aspects of retrosynthesis of simple-to-complex organic molecules.

Learning Outcomes

The students are expected to:

1. Acquire the knowledge and skills required to strategize and plan organic synthesis,
2. Develop an understanding of total synthesis of organic molecules.

Contents

Introduction: name reactions, functional group interconversions, transition metal catalyzed cross-coupling reactions, oxidations and reductions in organic synthesis (25 lectures)
Carbon-carbon bond formation: application of carbanions in organic synthesis, alkylation of enolates, enamines and hydrazones, alkylation of heteroatom stabilized anions, organometallic reagents and their application in synthesis (7 lectures)
Strategy and design of organic synthesis: scope and brief history of organic synthesis, synthetic strategy, concepts of synthetic equivalents and Umpolung, retrosynthetic analysis, linear and convergent synthesis, synthesis of 3-membered, 4-membered, 5 membered and 6-membered ring compounds (10 lectures)

Text books

1. Warren,S., and Wyatt.P., (2008), *Organic Synthesis: The Disconnection Approach*, 2nd Edition, Wiley-VCH
2. Nicolaou,K.C., Sorensen,E.J., (1996), *Classics in Total Synthesis: Targets, Strategies and Methods*, 1st Edition, Wiley-VCH
3. Carey,F.A., Sundberg,R.J., (2007), *Advanced Organic Chemistry, Part B: Reactions and Synthesis*, 5th Edition, Plenum

Reference Books

1. Clayden,J., Greeves,N., and Warren,S., (2012) *Organic Chemistry*, 2nd Ed., Oxford
2. Carruthers, W., (1989), *Some Modern Methods in Organic Synthesis*, Cambridge

Preparatory Course Material

1. Punniyamurthy,T., *Principles of Organic Synthesis*, NPTEL Course Material, Department of Chemistry, Indian Institute of Technology Guwahati, http://www.nptel.ac.in/courses/104103022/

Title	**Main Group and Bioinorganic Chemistry**	Number	CY522
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	M.Sc. (CY) Program	Type	Compulsory
Prerequisite			

Objectives

The Instructor will:

1. Give better insight into chemistry of main group elements and bioinorganic chemistry
2. Provide broad knowledge about properties and applications of compounds of main group elements and metal ions essential in biological systems.

Learning Outcomes

The students are expected to have the ability to:

1. Appreciate chemistry of elements essential in biological systems.
2. To understand structure and bonding concepts in chemistry of s- and p-block elements and systematic understanding of their chemical reactivity

Contents

Chemistry of main group elements: VSEPR and Point group symmetry, Synthesis, structure and bonding in polyhedral boranes and carboranes, Wade's Rules, electron count, Isolobal analogy. B-N, P-N, S-N unit containing compounds. Silanes, Silicon halides, Silicates, silanols, Zeolites. Hydrides, halides, oxides, nitrides of s- and p- block elements. Allotropes of Carbon. Chemistry of halogens and Noble gases, Acid-base concept, Chemistry of S-block elements. Organometallic compounds of main group elements. (15 Lectures)

Spectroscopic Characterization: NMR to study fluxionality and dynamic behavior in solution.(2 Lectures)

Applications of main group compounds: Frustrated Lewis pairs and 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) and ALD. (9 Lectures)

PET and SPECT imaging: *Overview of the development of radio-labelled p-block complexes for applications in PET and SPECT imaging* (2 Lectures)

Bioinorganic Chemistry: Transition metals in biology - their occurrence and function, active-site structure, Metalloenzymes; O2 binding properties of heme (hemoglobin and myoglobin) and non-heme proteins hemocyanin & hemerythrin), co-operativity effect, Bohr Effect; representative synthetic models of heme and nonheme systems. Electron transfer proteins - active site structure and functions of ferredoxin, rubredoxin and cytochromes, and their comparisons. Vitamin B12 and cytochrome P450 and their mechanisms of action. Metals in medicine. (12 Lectures)

Textbooks

1. Huheey, J. E., (2008), *Inorganic Chemistry*, 4th edition, Pearson
2. Housecroft, C. E., and Sharpe, A. G., (2012), *Inorganic Chemistry*, 4th Edition, Pearson
3. Miessler G. L., (2014), *Inorganic Chemistry*, 4th edition, Pearson

Reference Books

1. S. J. Lippard (1994) Principles of Bioinorganic Chemistry, University Science Books.
2. Norman, N. C., (2014), *Periodicity and the p-Block Elements*, Oxford Primer Nos. 51,2nd Edition, Oxford University Press
3. Atkins, P. (2010) *Inorganic Chemistry*, 5th Edition, Oxford University Press

Preparatory Course Material

1. Balakrishna, M. S., *Chemistry of Main Group Elements*, NPTEL Course Material, Department of Chemistry, Indian Institute of Technology Bombay, http://nptel.ac.in/courses/117101105/
2. Ray, D., *Bioinorganic Chemistry*, NPTEL Course Material, Department of Chemistry, Indian Institute of Technology, Kharagpur, http://nptel.ac.in/courses/104105031/

Title	**Transition Metal and Organometallic Chemistry**	Number	CY512
Department	Chemistry	Structure L-T-P[C]	3-0-0 [3]
Offered for	M.Sc. (CY) Program	Type	Compulsory
Prerequisite			

Objectives

The Instructor will:

1. To provide students with an overview of transition metal chemistry which form a foundation for students pursuing further studies in chemistry
2. To provide students fundamental of organometallic compounds and their practical applications.

Learning Outcomes

The students are expected to have the ability to:

1. Understand the properties and reactivites of selected transition metal complexes with their structure and bonding
2. Utilize the principles of transition metal coordination complexes in understanding reactivity and properties of organometallic compounds

Contents

Coordination Compounds: Survey of various ligands, coordination, thermodynamic stability, Isomerism, Irving-William series, chelate and macrocyclic effect. (5 Lectures)
Bonding in Coordination Complexes: VBT, CFT and MOT, Crystal Field Stabilization Energies and its applications, High and low spin complex, Jahn-Teller theorem. (8 Lectures)
Reaction mechanisms in Coordination complexes - substitution reactions in complexes, trans effect and its influence, water exchange, anation and base hydrolysis, stereochemistry, inner and outer sphere electron transfer mechanism (4 Lectures)
Spectroscopic properties: Colors, Selection rules. Splitting of the free ion energy levels in complexes. Term Symbol, Orgel, and Tanabe-Sugano diagrams. (6 Lectures)
Magnetic Properties: Origin of Magnetic moment, Effect of orbital contributions.(2 Lectures)
Bonding and properties of organometallic compounds: Ligands (carbonyl, olefins, phosphine, hydride, alkyls, carbines, carbenes). Compounds with carbonyl, olefins, EAN rule. Classification of ligands-sigma, pi-donor, pi-acceptor.(7 Lectures)
Bonding in organometallics: sigma and pi-back bonding, synthesis of organometallic compounds. Characterization by FTIR. (3 Lectures)
Organometallic Reaction and Catalysis: Oxidative addition, reductive elimination, CO insertion and migration reactions. Applications of Organometallic compounds in homogeneous catalysis – isomerization, hydrogenation, hydroformylation, Monsanto acetic acid synthesis, C-C coupling reactions, polymerization and metathesis. (6 Lectures)

Text Books

1. Weller, (2014), *Inorganic Chemistry*, 6th Edition, Oxford University Press
2. Huheey, J. E. (2006), *Inorganic chemistry: principles of structure and reactivity*, 4th Edition, Pearson
3. Crabtree, R. H. *The Organometallic Chemistry of the Transition Metals*, Wiley, 1998

Reference Books

1. Kettle, S.F.A., (2010), *Physical Inorganic Chemistry, A Coordination Chemistry Approach*, Springer
2. Housecroft, C and Sharpe, A. G. (2012) Inorganic *Chemistry*, 4th Edition, Pearson

Preparatory Course Material

1. Ray, D *Coordination Chemistry*, NPTEL course material, Department of Chemistry, Indian Institute of Technology, Kharagpur, http://nptel.ac.in/courses/104105033/
2. Samuelson, A.G., *Introduction to Organometallic Chemistry*, NPTEL Course Material, Department of Inorganic and Physical Chemistry, Indian Institute of Science, Bangalore, http://nptel.ac.in/courses/104108062/

Title	**Solid State and Material Chemistry**	Number	CY523
Department	Chemistry	L-T-P [C]	3-0-0 [3]
Offered for	M.Sc. (CY) Program	Type	Compulsory
Prerequisite			

Objectives

The Instructor will:

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

The students are expected to have the ability to:

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

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.(10 Lectures)
Crystal defects: non-stoichiometry, cluster, diffusion, Fick's Law and Kirkendall effect, Identification of defects using microscopic characterization techniques.(6 Lectures)
Solid state reaction: Chemical and Physical Methods of preparation, reactivity of solids, decomposition mechanism, single crystal growth and thin film deposition. (10 Lectures)
Band theory: Intrinsic and extrinsic semiconductors, insulators, density of states, Dielectrics, Hall effect, Thomson, Peltier and Seeback effects.(Lectures 8)
Properties of Solids: Magnetic, Electrical and Optical properties, Different type of Magnetism and Superconductivity, Introduction to nanomaterials and properties.(Lectures 6)

Textbooks

1. B. D. Cullity and S. R. Stock, (2014), *Elements of X-ray diffraction*, 3rd edition, Pearson
2. West, A.R., (2015), *Solid State Chemistry and Its Applications*, 2nd edition, John Wiley & Sons
3. Lesley E Smart and Elaine E Moore, (2005), *Solid State Chemistry: An Introduction*, 3rd Edition, Taylor and Francis
4. R. Balasubramaniam (2014), *Callister's Materials Science and Engineering*, 2nd Edition, Wiley

Reference Books

1. Cheetham, A.K. and Day, P., (1997), *Solid State Chemistry Compounds*, 2nd Edition, Clarendon Press, Oxford
2. Harry R. Allcock, (2008), *Introduction to Materials Chemistry*, 1st Edition, Wiley.
3. C N R Rao and J Gopalkrishnan, (2004) *New Directions in Solid State Chemistry*, 2nd Edition, Cambridge.

Preparatory Course Material

1. Subramaniam, A, *Structure of Materials*, NPTEL Course Material, Department of Materials Science and Engineering, Indian Institute of Technology Kanpur, http://nptel.ac.in/courses/113104014/16

Title	**Quantum Chemistry and Spectroscopy**	Number	CY514
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	M.Sc. (CY) Program	Type	Compulsory
Prerequisite			

Objectives

The Instructor will:

1. Attempt to provide an advanced level understanding of quantum chemistry
2. Will show a few applications of quantum mechanics to chemistry
3. Establish the relation between fundamentals of spectroscopy and quantum chemistry

Learning Outcomes

The students are expected to:

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

Contents

Fundamentals: Old Quantum theory, Correspondence principle, Bohr-Sommerfeld quantization, Wave-particle duality, Stern-Gerlach experiment (9 lectures)
Mathematical Formalism: Operators, Eigenfunctions and eigenvalues, Operators in quantum mechanics, expectation values, Theorems of Quantum Mechanics, Commuting and non-commuting operators, Angular momentum (10 lectures)
Exactly Solvable Problems: Time independent and time dependent wave equation, Particle confined to infinite and finite potential wells, Harmonic oscillator, Rigid rotor, Hydrogen atom (10 lectures)
Approximation Methods: Variational principle, Perturbation theory, Energy and wave function corrections, Born-Oppenheimer approximation (8 lectures)
Introduction to spectroscopy: Introduction to rotational, vibrational spectroscopy, electronic transitions, Frank-Condon principle, vertical transitions – selection rules, parity, symmetry and spin selection rule (5 lectures)

Textbooks

1. Levine, I. N., (1983), *Quantum Chemistry*, 3rd Edition, Allyn and Bacon

Reference Books

1. McQuarrie,D. A., (1983), *Quantum Mechanics*, 2nd Edition, University Science Books
2. Bernath,P. F., (2005), *Spectra of Atoms and Molecules*, 2nd Edition, Oxford University Press, London
3. Banwell,C. N., (2010), *Fundamentals of Molecular Spectroscopy*, 4th Edition, Tata McGraw Hill, New Delhi

Preparatory Course Material

1. Krishnan, M. S., *Introduction to Quantum Chemistry and Molecular Spectroscopy*, NPTEL Course Material, Department of Chemistry, Indian Institute of Technology Madras, http://nptel.ac.in/courses/104106083/

Title	**Molecular Thermodynamics and Chemical Kinetics**	Number	CY513
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	M.Sc. (CY) Program	Type	Compulsory
Prerequisite			

Objectives

The Instructor will:

1. Provide the connection between microscopic theory and thermodynamics.
2. Describe how complex phenomena can be transferred into simple models.

Learning Outcomes

The students are expected to:

1. Predict properties of many-body systems starting from its microscopic constituents and their interactions
2. Connect microscopic theory to chemical reaction

Contents

(fractal 1, Thermodynamics and Enzyme Kinetics by BSBE) *Thermodynamics:* thermodynamics laws, state and path functions and their applications; thermodynamic description of various types of processes; Maxwell's relations; spontaneity and equilibria (5 lectures)
temperature and pressure dependence of thermodynamic quantities; Le Chatelier's principle (5 lectures).
(Module 3 of Applied Thermodynamics by ME) *Introduction to Statistical methods:* Micro and macro states, canonical, micro canonical and grand canonical ensemble, Boltzmann distribution; kinetic theory of gases; partition functions, thermodynamic properties from partition functions for model systems; Debye-Huckel theory (12 lectures).
(fractal 1, Thermodynamics and Enzyme Kinetics by BSBE) *Chemical Kinetics:* Empirical rate laws and temperature dependence; complex reactions; steady state approximation, enzyme kinetics ; determination of reaction mechanisms (10 lectures)
Mechanism: Theory of reaction rates, activation energy, transition state theory, potential energy surface, uni-molecular reaction rate, salt effects (10 lectures).

Text Books

1. D. McQuarrie and J. D. Simon, (2014) *Molecular Thermodynamics*, Viva Books.
2. D. McQuarrie, (2011) *Physical Chemistry, A Molecular Approach*, Viva Books.

Self Learning Material

1. D. McQuarrie, (2000) *Statistical Mechanics*, University Science Books.
2. K. J. Laidler, (2013) Chemical Kinetics, Pearson.

Preparatory Course Material

1. V.Balakrishnan, Department of Physics, IIT Madras. http://nptel.iitm.ac.in
2. Leonard Susskind, Statistical Mechanics, Stanford University, https://www.youtube.com/watch?v=D1RzvXDXyqA&t=901s
3. De, A. K. *Advanced Chemical Thermodynamics and Kinetics*, NPTEL Course Material, Chemical Sciences, IISER Mohali, https://onlinecourses.nptel.ac.in/noc18_cy20/

Title	**Theory and Applications of Spectroscopic Techniques**	Number	CY5xx
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	M.Sc. (CY) Program	Type	Compulsory
Prerequisite			

Objectives

The Instructor will:

1. Introduce to a few spectroscopic methods used as analytical techniques in various fields of science and engineering.
2. Introduce to theoretical background of these methods along with their instrumentation and application.

Learning Outcomes

The students are expected to:

1. Understand the theoretical background of various spectroscopic techniques.
2. Apply spectroscopic methods as analytical tool in chemistry, biology, material science, medicine.

Contents

Introduction to Spectroscopy: properties of electromagnetic radiation, interaction of radiation with matter, Stimulated and Spontaneous processes, Einstein coefficient, Rabi Oscillation, intensity of spectral line and line shape, Fourier Transformation, General understanding of spectroscopic selection rule (6 lectures)
UV-vis and Fluorescence Spectroscopy: Basic principles, Laws of photochemistry, Jablonski diagram, Frank-Condon principle, quantum yield expression and Stern-Volmer equation, FRET. (8 lectures)
Infrared and Raman Spectroscopy: Basic principle; Organic functional group identification through IR spectroscopy, IR and Raman activity. (12 lectures)
NMR Spectroscopy: Basic principle, Zeeman splitting, chemical shift and spin-spin coupling, introduction to AB, AX, AMX spin system, 1D 1H and 13C NMR for structure elucidation, Polarization transfer methods and NOE (10 lectures)
EPR Spectroscopy: basic principle, Electron-nuclear hyperfine interaction, theory of first order EPR spectra, analysis of 1st Order spectra, example of EPR spectra of organic radicals and transition metal complexes. (5 lectures)

Textbooks

1. Gunther, H., (1995), *NMR Spectroscopy*, 2nd Edition, Wiley
2. Banwell, C. N., (1994), *Fundamentals of Molecular Spectroscopy*, 3rd Edition, Tata McGraw-Hill Book Company
3. Lakowicz, J. R., (2006), *Principles of Fluorescence Spectroscopy*, 3rd Edition, Springer, New York

Reference Books

1. Bernath, P. F., (2005), *Spectra of Atoms and Molecules*, 2nd Edition, Oxford University Press
2. Silverstein, R. M. and Webster, F. M., (2010), *Spectroscopic Identification of Organic Compounds*, 6th Edition, Wiley

Preparatory Course Material

1. Mangal Sundar, K., *Introduction to Quantum Chemistry and Molecular Spectroscopy,* http:// http://nptel.ac.in/courses/104106083
2. Trivedi, V. and Chaudhary, N., *Bioanalytical Techniques and Bioinformatics*, Department of Biotechnology, http:// http://nptel.ac.in/courses/ 102103044.
3. Das, R., *Principles and Applications of Electron Paramagnetic Resonance Spectroscopy*, Department of Chemical Sciences, https://nptel.ac.in/courses/104106048/2

Laboratories and Hands-on

Title	**Organic Chemistry Laboratory**	Number	CY5XX
Department	Chemistry	L-T-P [C]	0–0–3[1.5]
Offered for	M.Sc. (CY) Program	Type	Compulsory
Prerequisite			

Objectives

The instructor will:

1. Give students a practical understanding of the theoretical phenomenons.
2. Provide an exposure to the laboratory techniques for the purification and isolation of organic compounds

Learning Outcomes

The students are expected to:

1. Learn basic experimental techniques in organic chemistry
2. Be able to carry out simple synthetic organic transformations and isolate the reaction products

Contents

Extraction: separation of an acidic, a basic and a neutral substance
Thin Layer Chromatography (TLC): extraction and TLC of spinach pigments
Hands on Reactions and Purifications by Column Chromatography: Wittig olefination, Henry reaction (Nitro-Aldol reaction), Grignard reaction etc..
Distillation: Separation of compounds based on boiling point
Elimination Reaction: Dehydration of methylcyclohexanols to methylcyclohexene
Cycloaddition: The Diels-Alder reaction of a conjugated diene either in eucalyptus oil or other dienophiles
Aromatic Substitution: The Friedel-Crafts acylation of ferrocene
Functional Group Interconversion: Reduction and oxidation of organic compounds
Drug Synthesis: Synthesis of Aspirin from Salicylic Acid
Green Chemistry: A Solvent-Free Aldol Condensation

Textbook

1. Vogel, A. I., *Textbook of Practical Organic Chemistry*, Pearson

Reference Books

1. Ault, A., *Techniques and Experiments for Organic Chemistry*, University Science Books

Title	**Inorganic Chemistry Laboratory**	Number	CY5XX
Department	Chemistry	L-T-P [C]	0-0-3 [1.5]
Offered for	M.Sc.(CY) Program	Type	Compulsory
Prerequisite			

Objectives
The Instructor will:
1. Emphasize on the different techniques of reaction set-up (air-sensitive, moisture-sensitive etc. involved in the synthesis, isolation and purification of inorganic compounds.
2. Expose students to various spectroscopic identification and characterization techniques.

Learning Outcomes
The students are expected to have the ability to:
1. Understand the basic principles behind the synthesis and properties of inorganic compounds.
2. Plan and Conduct experiments for synthesis and characterizing inorganic compounds.

Contents
Laboratory Experiments:

Non-metal complex: Synthesis and characterization of bispyridine iodide nitrate; Solid phase synthesis and characterization of trans-bis glycinato copper(II); Synthesis of penta amminechlorocobalt(III)chloride and its spectroscopic properties; Influence of ligand field tetragonality on the ground state spin of nickel(II) complexes with NH_3 and H_2O and ethylene diamine; Preparation and magnetic properties of Fe^{III}(acac) complex; Preparation of TiO_2 from Titanium Isopropoxide; Preparation and Characterization of Hydroxyapatite; Luminescent Ruthenium Complexes. Synthesis of $RuHCl(CO)(PPh_3)_3$ complex and its characterisation by 1H, 31P NMR and IR spectroscopy

Text Books
1. G. S. Girolami, T. B. Rauchfuss, R. J. Angelici *Synthesis and Technique in Inorganic Chemistry,* University Science Books*, 3rd Ed,* 1999.
2. Elias, A. J., A Collection of Interesting General Chemistry Experiments, Universities Press(India) Pvt. Ltd., 2002

Reference Books
1. J. Derek Woolins, Inorganic Experiments, 3^{rd} Edition, Wiley, 2010.
2. Roesky, H. W.; Muckel, K., Chemical Curiosities: spectacular experiments and inspired quotes, VCH, 1996.
3. Handouts prepared for the laboratory experiments: collections from various literature sources (ACS Chemical Education)

Self Learning Material
John Dolhun. 5.301 Chemistry Laboratory Techniques. January IAP 2012. Massachusetts Institute of Technology: MIT Open Courseware, https://ocw.mit.edu.

Course Title	**Physical Chemistry Laboratory**	Course No.	CY5xx
Department	Chemistry	L-T-P [C]	0-0-3 [1.5]
Offered for	M.Sc. (CY) Program	Type	Compulsory
Pre-requisite			

Objectives

The instructor will:
1. Introduction to the different spectroscopic and analytical techniques.
2. Introduction to the instrumentation and application of these methods.
3. Enable students to use such methods whenever needed by giving hands on experience with available instruments in the institute.

Learning Outcomes

The students are expected to:
1. Clear understanding of different analytical instruments.
2. Experimental verification of fundamental concept
3. Application of spectroscopic techniques as analytical tool in chemistry.

Course Content
1. Determination of the pI of an Amino Acid using pHmeter.
2. Determination of critical micellar concentration by conductometry and calculation of free energy of micellization
3. Determination of Heat Capacity of metals by Dynamic Scanning Calorimeter and verification of Dulong and Petit Method
4. Determination of the ligand-protein binding constant using Fluorescence quenching technique
5. Determination of ^{1}H spin-lattice relaxation time by NMR Inversion Recovery method
6. Determination of Gibbs free energy of the keto-enol tautomerism by ^{1}H NMR
7. Determination of bromobenzene surface coverage on silica by FTIR
8. Study of surface properties (surface energy and surface tension) of various surfaces and solutions.
9. Study of Redox reactions for understanding the reversibility of the reactions using cyclic voltammetry
10. Surface Adsorption Kinetics of Dyes on activated carbon using UV-Visible spectroscopy/calorimetry

Text Books
1. Halpern, A. M.; McBane, G. C. Experimental Physical Chemistry: A laboratory Textbook, 3rd ed. W. H. Freeman, 2006.

Reference Books

Literature papers from ACS Chemical Education

Title	**Computational Chemistry Laboratory**	Number	CY 5xx
Department	Chemistry	L-T-P [C]	0-0-3 [1.5]
Offered for	M.Sc. (CY) Program	Type	Compulsory
Pre-requisite	CY 524 (Chemical Binding)		

Objectives

The Instructor will:

1. Provide the connection between theory and experiments
2. Provide the understanding of how complex phenomena can be transferred into simple models.

Learning Outcomes

The students are expected to:

1. Learn tools and techniques used in computational chemistry.
2. Develop computational skills related to chemistry.

Contents

1.Drawing the geometry of a molecule - Read XYZ coordinates - measure bond distances and angles (MOLDEN).

2.Using a fixed nuclear geometry, compute the ground state electronic energy of a molecule using Hartree-Fock, MP2, and DFT.

3.Perform geometry optimization (energy minimization) using different theories.

4.Compute the vibrational frequencies and differentiate a minimum and a saddle point.

5.Calculate potential energy profile and intrinsic reaction coordinate of a reaction.

6.Learn visualizing bulk system using computer (VMD).

7.Build bonded and non-bonded potential parameters after geometry optimization.

8.Energy minimization of a bulk system at meso-scale.

9.Different ensembles, NVT, NPT, NVE.

Text Books

1. Levine, I. N., (1983), *Quantum Chemistry*, 3rd Edition, Allyn and Bacon
2. Molecular Modelling: Principles and Applications, Andrew Leach, 2nd Edition, Pearson.
3. Daan Frenkel and Berend Smit, (2002) Understanding Molecular Simulation, Academic Press.

Reference books

1. Mark E. Tuckerman, *Statistical Mechanics, (2010) Theory and Molecular Simulations*, Oxford University Press.
2. Szabo, A.and Ostlund, N.S. (1996), Modern Quantum Chemistry, Dover.

Course Title	**Hands on -1**	Course No.	CY5xx
Department	Chemistry	L-T-P [C]	0-0-3 [1.5]
Offered for	M.Sc. (CY) Program	Type	Compulsory
Pre-requisite			

Objectives

The instructor will:

1. Provide the students hands-on training using the available characterization tools .
2. Provide students with the knowledge and skills needed to conduct laboratory research, understand instrument design and analyze instrumental results.

Learning Outcomes

The students are expected to:

1. Have clear understanding of different analytical instruments.
2. Experimental verification of fundamental concept
3. Application of spectroscopic techniques as analytical tool in chemistry.

Course Content

1. Chromatographic Techniques (GC and HPLC) in Organic Analysis
2. Fluorescence Spectroscopy and its application
3. Synthesis techniques and laboratory practices
4. OriginPro Data Analysis and Plotting of graphs
5. MERCURY and ENCIFER Crystal structure viewing
6. MATLAB for data analysis: basic plotting techniques; curve fitting; and simple linear programming;
7. Chem Draw for drawing molecular structures
8. Mathematica for mathematical data handling
9. Technical communication - presentation, literature search
10. Scifinder for literature search
11. Analysis and identification of organic compounds by 1H NMR, Mass spectrometry and IR
12. Modeling of intermediate and transition state of organic reactions

Text Books:

1. Halpern, A. M.; McBane, G. C. Experimental Physical Chemistry: A laboratory Text Book, 3^{rd} ed. W. H. Freeman, 2006.

Reference Book:

1. Online resources from ACS Chemical Education
2. Hunt, B. R. et al., A guide to MATLAB: For beginners and experienced user, 2nd Edition, University Press, Cambridge, 2006
3. ChemDraw user guide: http://media.cambridgesoft.com/support/15/ChemDrawHelp.pdf
4. McMahon, D, A & Topa, D. M., A beginners guide to Mathematica, Chapman & Hall/CRC, 2006.

Course Title	**Hands On -2**	Course No.	CY5xx
Department	Chemistry	L-T-P [C]	0-0-3 [1.5]
Offered for	M.Sc. (CY) Program	Type	Compulsory
Pre-requisite			

Objectives

The instructor will:

1. Provide the students hands-on training using the available characterization tools .
2. Provide students with the knowledge and skills needed to conduct laboratory research, understand instrument design and analyze instrumental results.

Learning Outcomes

The students are expected to:

1. Clear understanding of different analytical instruments.
2. Experimental verification of fundamental concept
3. Application of spectroscopic techniques as analytical tool in chemistry.

Contents

1. NMR Working principles and instrumentation
2. Single Crystal X-Ray Diffraction Working principles and instrumentation
3. Electroanalytical Methods (Ampereometry, Cyclic Voltametry, EIS spectroscopy etc)
4. SEM Working principles and instrumentation
5. AFM Working principles and instrumentation
6. UV-Vis Working principles and instrumentation
7. IR Working principles and instrumentation
8. TGA/DSC Working principles and instrumentation
9. BET Surface Area Analyser Working principles and instrumentation
10. PXRD Working principles and instrumentation

Text Books

1. Halpern, A. M.; McBane, G. C. Experimental Physical Chemistry: A laboratory Text Book, 3rd ed. W. H. Freeman, 2006.

Reference Book:

1. Literature References from ACS Chemical Education

Electives

Title	**Catalysis for Energy**	Number	CY6xx
Department	Chemistry	L-T-P [C]	3-0-0 [3]
Offered for	MSc./PhD (CY) Program	Type	Elective
Prerequisite			

Objectives
The Instructor will:
1. To give a overview about defining a roadmap for the role of catalysis in energy production
2. Relate catalysis with fuel cells, hydrogen production and storage, methane storage and industrial catalysis

Learning Outcomes
The students are expected to have the ability to:
1. Understand role and the possibilities of catalysis in the production of new energy carriers and in the utilization of different energy sources.
2. to go beyond conventional application identifying new developments that may lead to breakthroughs in the production of alternative energy.

Contents
Catalysis: Introduction to heterogeneous catalysis, including models of surface reactivity, surface equilibria, kinetics of surface reactions, electronic and geometrical effects in heterogeneous catalysis.(Lectures 14)
Catalytic reactions and application: Trends in reactivity, catalyst structure and composition, electro-catalysis and photo-catalysis.(Lectures 12)
Selected applications and challenges in energy transformations: fuel cells, hydrogen production, OER and HER reactions, CO_2 oxidation, methane and hydrogen storage and industrial catalysis. (Lecture 14)

Textbooks
1. Hanefeld, U, Lefferts, L. (2018) Catalysis: An Integrated Textbook for Students, 1st Edition, Wiley

Reference Books:
1. Okada, Tatsuhiro, Kaneko, Masao, (2009), *Molecular Catalysts for Energy Conversion* Springer.
2. Guczi, László, Erdôhelyi, András, *Catalysis for Alternative Energy Generation*, Springer.
3. Pierluigi Barbaro, Claudio Bianchini, *Catalysis for Sustainable Energy Production,* Wiley

Self Learning Material
1. Xile Hu, Angamuthu, R and Bera, J. K., Catalysis for Energy Storage, GIAN Course material, Indian Institute of Technology Kanpur, https://www.youtube.com/watch?v=LvTfsIAI-VE

Title	**Nanomaterials and Nanodevices**	Number	CY653
Department	Chemistry	L-T-P [C]	2-0-1 [3]
Offered for	MSc/PhD (CY) Program	Type	Elective
Prerequisite			

Objectives

The Instructor will:

1. Underlying scientific basis for the behavior of nanomaterials
2. Methods of synthesis, fabrication and characterization of nanomaterials
3. Scope of nanomaterials and potential translation as products

Learning Outcomes

The students are expected to have the ability to:

1. Able to describe the basic science behind the properties of materials at the nanometer scale
2. Learn principles behind advanced experimental techniques for studying nanomaterials
3. Systematically solve scientific problems related specifically to Nano technological materials

Contents

Concepts, Definitions and Examples: Nanoscale processes, nanosystems, nanostructures, important nanomaterials such as clusters, nanocrystals, nanotubes and nanowires. (2 Lectures)
Size-dependent properties: Quantum confinement, Bandgap, Surface effects in nanosystems. Optical, mechanical, electronic and magnetic properties along with surface reactivity.(6 Lectures)
Synthesis of nanomaterials: Top-down and bottom-up, soft versus hard methods, chemical and physical methods, hybrid methods for synthesis of nanomaterials.(6 Lectures)
Experimental methods for study of nanomaterials: Electron microscopes (SEM and TEM), scanning probe microscope (AFM and STM), X- ray photoelectron spectroscopy, BET surface area, electroanalytical techniques and miscellaneous methods (6 Lectures)
Nanolithography for Nanodevices: Concepts and methods; fabrication of devices, clean room practices, optical, electron, ion- beam lithography, soft lithography, micromolding, nanoimprint lithography. (6 Lectures)
Applications: Translating nanomaterials and nanodevices as commercial products.(4 lectures)

Laboratory Experiments

Synthesis of metal nanoparticles, Particle size analysis by UV Visible spectroscopy, synthesis of semiconducting ZnO nanoparticles, quantum dots, optical band gap analysis by emission spectrum, SEM imaging, AFM analysis, patterning by Photo/Soft Lithography,graphene synthesis and surface property analysis

Text Books

1. Pradeep, T., (2012), *Textbook of Nanoscience and Nanotechnology*, Mc Graw Hill
2. C. N. R. Rao, P. J. Thomas and G. U. Kulkarni (2007)Nanocrystals: Synthesis, Properties and Applications,Springer.

Reference Books

1. Nalwa, H. S., (2004), *Encyclopedia of Nanoscience and Nanotechnology*, Edition American Scientific Publishers, Los Angeles
2. Rao, C.N.R. and Govindaraj, A., (2005), *Nanotubes and nanowires*, RSC Publishing
3. C. N. R. Rao, P. J. Thomas and G. U. Kulkarni (2007)Nanocrystals: Synthesis, Properties and Applications,Springer.

Preparatory Course Material

1. Subramaniam, A., Balani, K. *Nanostructures and Nanomaterials: Characterization and Properties*, NPTEL Course Material, Department of Materials Science & Engineering, Indian Institute of Technology, Kanpur, http://nptel.ac.in/courses/118104008/;

Title	**Compounds of p-block elements and Applications**	Number	CY6XX
Department	Chemistry	L-T-P [C]	3-0-0 [3]
Offered for	M.Sc./PhD (CY) Program	Type	Elective
Prerequisite			

Objectives

The Instructor will:

1. To give better insights into the interesting class of compounds such as rings, clusters, polymers and low valent complexes of the main-group elements.
2. To learn about the synthesis, structure and properties of inorganic heterocyclic and homocyclic rings.
3. To discuss about structure, properties and reactivity of clusters and cages of main group elements.

Learning Outcomes

The students are expected to:

1. Appreciate the interesting class of compounds such as rings, clusters and polymers of main group metal compounds.
2. Gain deeper insights into the synthesis and reactivity of novel main group compounds.
3. Understand structure-property relationships and applications of inorganic, organometallic polymers and low valent compounds.

Contents

Inorganic Rings: Synthesis, structure and reactivity of compounds containing heterocyclic rings of elements such as Phosphorus, Boron, Silicon, Tin and Aluminum. Structure and reactivity of compounds containing homocyclic rings of germanium, boron, silicon, aluminum. Synthesis and properties of inorganic macrocycles. (10 Lectures)
Clusters: Clusters and Cages of Main Group Elements, Boron Hydrides and Carboranes. Homo and Heteropolyatomic Anions of the Post-Transition Elements. (8 Lectures)
Inorganic polymers: Synthesis, structure-property relationships and applications of Polysiloxanes, Polyphosphazenes, polysilanes and organometallic polymers. (10 Lectures)
Chemistry of Low valent compounds: Low valent compounds of main group elements, Recent advances in NHCs and their analogous group 13, 14 and 15 compounds. (6 Lectures)
Applications: Main group element containing rings, clusters and polymers as single source precursors for nanomaterials. Low valent compounds in small molecule activation. (9 Lectures)

Textbook

1. Chivers, T. and Manners, I., (2009), Inorganic Rings and Polymers of the p-Block Elements, 1st Edition, Royal Society of Chemistry

References

1. R. D. Archer, (2001), Inorganic and Organometallic Polymers, Wiley
2. H. R. Allcock, (2003), Chemistry and Applications of Polyphosphazenes, Wiley
3. V. Chandrasekhar, (2005), Inorganic and Organometallic Polymers, Springer-Verlag
4. M. Driess, (2004), Molecular Clusters of the Main Group Elements, Wiley-VCH
5. P. Atkins, (2008), Inorganic Chemistry, Indian Edition, 4th Ed, Oxford University Press

Preparatory Course Material

1. Balakrishna, M. S., *Chemistry of Main Group Elements*, NPTEL Course Material, Department of Chemistry, Indian Institute of Technology Bombay, http://nptel.ac.in/courses/117101105/

Title	**Advanced Materials Design**	Number	CY7xx
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	M.Sc./PhD (CY) Program	Type	Elective
Prerequisite			

Objectives

The Instructor will:

1. Provide a comprehensive overview of synthesis and characterization of bulk materials, nanoparticles, nanocomposites and hierarchical materials with nanoscale features.
2. cover the fundamental scientific principles controlling assembly of nanostructured
3. materials; synthesis, characterization tools; new properties at the nanoscale, and
4. existing and emerging applications of nanomaterials

Learning Outcomes

The students are expected to:

1. Understand a variety of different methods for synthesizing materials.
2. Evaluate the synthesis methods against each other and be able to make assessments as to what form the final products will be.
3. Should be able to assess appropriate methods for the synthesis of stable nanomaterials

Contents

Introduction to Materials Chemistry: Structure, property and their relationship with materials performance (3 Lectures)

Semiconducting Materials Chemistry: Semiconductor Devices, Phase Change Materials in Memory Technology, Thermoelectric, Superconductors, Topological Insulators, Emerging materials in the device industry such as graphene and 2D materials.(8 Lectures)

Optical/Opto-electronic Materials: Light Emitting Diodes, Photosensors, Photovoltaics (6 Lectures)

Structural & Basic Applied Materials: Structural Materials, Amorphous Materials, Smart & Responsive Materials, Bio-inspired materials (8 Lectures)

Thermal Materials Application: Thermochromics (2 Lectures)

Energy Materials: Batteries and Supercapacitors, Fuel Cells,Hydrogen generation,Hydorgen storage, Carbon capture and sequestration (12 Lectures)

Student Seminars on Selected Topics from above

Textbooks

1. Fahlman, Bradley, (2011), Materials Chemistry, 3rd Edition, Springer
2. P. Yang (2003), The Chemistry of Nanostructured Materials, 1st Edition, World Scientific Publishing Company, Singapore

Reference Books

1. G. Cao, (2004), Nanostructures and Nanomaterials: Synthesis, Properties and Applications, Imperial College Press: Hackensack, NJ
2. Goldstein, J.I. *et al.* (1992), *Scanning Electron Microscopy and X-Ray Microanalysis: A Textbook for Biologists*, Materials Scientists and Geologists, 2nd Edition, Springer, US.

Preparatory Course Material

1. Qureshi, M. *Chemistry of Materials*, NPTEL Course Material, Indian Institute of Technology Guwahati, http://nptel.ac.in/courses/104103019/2

Course Title	**Characterization Techniques in Inorganic Chemistry**	Course No.	CY 6xx
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	M.Sc/PhD Program	Type	Elective
Pre-requisite			

Objectives

The instructor will:

1. To provide introduction to various characterization methods that are applied to inorganic chemical systems.

Learning Outcomes

The students are expected to:

1. Appreciate different important characterization methods that are applied to inorganic chemical systems.
2. Analyze the chemical and physical characterization of molecular (solution and solid-state) inorganic chemical systems.

Contents

Fundamental aspects of characterisation methods in inorganic chemistry.

Molecular Symmetry: Point group analysis of simple inorganic 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. (6 Lectures)

Electronic spectroscopy: electronic absorption and emission spectroscopy (4 Lectures)

Multinuclear NMR: Use of 1H and 13C NMR to study fluxionality and dynamics in inorganic and organometallic chemical systems; NMR spectral analyses of B, Al, Si, F, and P containing compounds. Inorganic and Organometallic compounds of some other NMR active nuclei will also be discussed. (11 Lectures)

EPR: Elementary aspects of Electron paramagnetic resonance (EPR) spectroscopy of inorganic compounds- g-values, hyperfine and super hyperfine coupling constants; selected applications in inorganic chemistry. (5 Lectures)

Mass spectrometry: basic principles, ionization techniques, isotope abundance, molecular ion; illustrative examples from supramolecules, inorganic/coordination and organometallic compounds. (5 Lectures)

X-ray and Photoelectron Spectroscopy: *Electron microscopy and energy dispersive analysis of X-rays (5 Lectures)*

Cyclic voltammetry: Introduction to cyclic voltammetry and discussion on cyclic voltammogram of some representative examples. (5 Lectures)

Text Books

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

Reference Books

1. M. Weller, Inorganic Chemistry, 6th Edition, Oxford University Press, 2014.
2. J. E. Huheey, Inorganic Chemistry, Principles of Structure and Reactivity, 4th Edition, Pearson, 2006.
3. F. A. Cotton, 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)

Preparatory Course Material

1. Alagarsamy P, *Characterization of Materials* NPTEL Course Material, Department of Chemistry, Indian Institute of Technology Guwahati,https://nptel.ac.in/courses/115103030/

Course Title	**Advance Catalysis**	Course No.	CY6XX
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	MSc/PhD (CY) Program	Type	Elective
Pre-requisite			

Objectives

The instructor will:

1. Provide knowledge of key aspects of organometallic chemistry including the different binding modes of organic ligands, variation in oxidation states and electron counts.
2. Provide an understanding of the fundamental types of organometallic reaction, such as insertion, oxidative-addition

Learning Outcomes

The students are expected to:

1. understand some fundamental organometallic transformations that underpin the catalytic formation of carbon-containing species.
2. understand basic knowledge, skills and experience useful to those students progressing into the chemical industry and research in the area of catalysis

Course Contents

*Fundamentals of Catalysis :*Definition, reaction coordinate diagram, homogeneous catalysis, mechanism, catalytic cycle, fundamental organometallic processes, ligand substitution, oxidative addition, migratory insertion, transmetallation, reductive elimination, transition metals versus homogeneous catalysts, turnover limiting step, features of a catalytic process, Effective Atomic Number Rule (18-electron-rule). (8 Lectures)

Stereochemistry and Selectivity: Concepts and Definitions, Isomers, constitution, configuration enantiomers and diastereomers, conformation, stereochemical terms-a primer, optical activity, methods for determination of enantiomeric excess-chiral stationary phase (CSP) GC and CSP-HPLC and NMR. (8 Lectures)

*Consequences of diastereoisomerism: (*i) resolution of enantiomers via formation of diastereomeric salts, (ii) resolution via chromatography (GC and HPLC), (iii) identification of absolute stereochemistry, (iv) determination of enantiomeric ratio (er), or enantiomeric excess (ee), NMR shift reagents, (iv) diastereoselective synthesis, (v) kinetic resolution, examples and (vi) enantioselective synthesis, examples. (7 Lectures)

Hammond Postulate: Kinetic and Thermodynamic Control. Kinetic and thermodynamic control, use of energy diagrams, examples: DBr addition to 1,3-butadiene, enolate formation from 2-methylcyclohexanone, Hammond postulate, examples: Markovnikov regioselectivity of HX addition to monosubstituted alkenes, Orientation in electrophilic aromatic substitution reactions (7 Lectures)

Asymmetric Catalysis Using Organometallic Reagents: Hammond Postulate and Curtin Hammett Concepts, Methods and Origin of Selectivity. CurtinHammett principle,reactivity ofconformations pyrolytic elimination, Felkin-Anh model for predicting acyclic stereoselection, [Rh(L*)]+ X− , L* =chiral ligand)]-catalyzed asymmetric hydrogenation of dehydroamino-acids for the synthesis of enantiopure alpha-amino-acids Diastereomeric intermediates and origin of selectivity, Pd(0)-catalyzed allylation of stabilized carbon nucleophiles and Rh Catalyzed hydrogenation two classical examples with different reaction profiles (10 Lectures)

Text Books

F A Cotton, G. Wilkinson, C A Murillo and M Bochmann, *Advanced Inorganic Chemistry*, 6th ed, 1999, WileyInterscience

C Elschenbroich and A Salzer, *Organometallics*, VCH Publishers, 1st ed 1989, 2nd ed 1993.

R H Crabtree, *The Organometallic Chemistry of the Transition Metals*, Wiley, 1998

C Masters, Homogeneous Transition-metal Catalysis - A Gentle Art, Chapman and Hall, 1981

Course Title	**Water Chemistry**	Course No.	CY6XX
Department	Chemistry	L-T-P [C]	2–0–1 [3]
Offered for	BTech/MTech/MSc/PhD(CY) Program	Type	Elective
Pre-requisite	*Consent of Teacher*		

Objectives

The instructor will:

1. Provide the objective of this course is to provide a fundamental and advance understanding of the chemical and biochemical processes that are involved in water treatment for drinking purposes and treatment of industrial and domestic wastewaters for water reuse and discharge to the environment
2. Provide knowledge of the key chemical processes relevant to research in water chemistry

Learning Outcomes

The students are expected to:

1. Perform quantitative and qualitative interpretations for water quality analysis
2. Apply concepts of chemical equilibrium to solve water related practical problems

Course Contents

Polar nature of water: Acids and bases, Buffering capacity of water (3 Lectures)
Equilibrium constant expressions: aqueous system including concentration, activities, activity coefficients and pH of equilibrium. (4 Lectures)
Chemical reaction equation: Arrenhius and Bronsted-Lowry acids and bases (4 Lectures)
Ionization constant reactions and expressions: Self-Ionization of water, Solubility-product expressions (4 Lectures)
Measurments: pH, Filtration, Alkalinity and aqueous titrations (3 Lectures)
Cycling of water and residence time (3 Lectures)
Water availability, usage, quality: water treatment methods (5 Lectures)
Analytical methods for water quality analysis (6 lectures)

Laboratory Experiments

Measuring color in water, removing turbidity, acidity determination, alkalinity determination, chloride in water, hardness test for water, dissolved oxyzen by winkler's method

Reference Books

Sawyer, C., McCarty, P., & Parkin G, *Chemistry for Environmental and Engineering Science*. 5th Edition. Toronto: McGraw-Hill, 2003

Mark M. Benjamin, 2015, Water Chemistry, Waveland Press, Second Edition, ISBN 1-4786-2308-X

Text Books

Werner Stumm, James J. Morgan, *Aquatic Chemistry: Chemical Equilibria and Rates in Natural Waters, 3rd Edition*, Wiley

Kerry J. Howe, David W. Hand, John C. Crittenden, R. Rhodes Trussell, *Principles of Water Treatment*, George Tchobanoglous, Wiley

Preparatory Course Material

1. NPTEL Lectures: https://nptel.ac.in/courses/122106030/

Title	**Frontiers in Organometallic Catalysis**	Number	MT6XX
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	M.Sc. and Ph.D	Type	Elective
Prerequisite	Consent of teacher		

Objectives

1. To impart advanced knowledge on frontiers of organometallic chemistry.
2. To teach practical applications of organometallic compounds in homogeneous catalysis particularly relevant to industrial applications.

Learning Outcomes

1. The learners are expected to gain knowledge of independent thinking in designing, characterizing and fine tuning of organometallic complexes suitable for potential catalytic transformations.
2. Learners will be able to delineate mechanistic proposal of catalytic reactions based on available experimental data.
3. Learners will have the update on current trends and challenges of organometallic chemistry towards molecular activation and organic transformations focusing on sustainable development.

Contents

Introduction: Basics of organometallics, 18 e- rule, sigma and pi donor/acceptor ligands (5 lectures)

Synthetic, characterization and reactivity strategies of Transition Metal hydrides bearing carbonyl, nitrosyl, carbene, phosphine, olefins, and so on as ancillary ligands. Inert bonds (C-H, C-C, O-H, N-H) and small molecules (H_2, CO, CO_2) activation mediated by organometallic complexes. (12 lectures)

Definition and concepts of catalysis: Important terminologies in catalysis Hydrogenation, dehydrogenation, dehydrogenative coupling reactions, hydrosilylation, hydroformylation, hydroamination, hydrocyanation, hydrozirconation, carbonylation, Wacker oxidation, Fischer Tropsch synthesis, water gas shift reaction, Olefin polymerisatization, olefin metathesis, Mechanistic pathway interpretation: Kinetic studies, Deuterium Kinetic Isotope effect, Rate limiting step, Resting state, Scrambling experiments. (13 lectures)

Approaches towards Sustainability using organometallic complexes: Pincer catalysts design, Utilization of CO_2 and other feed stocks; Sustainable Energy: H_2 economy, Methanol economy, Liquid organic hydrogen carrier. (6 lectures)

Frustrated Lewis pair Chemistry: Hydroboration, carboboration, small molecule activation, catalysis. (5 lectures)

Textbooks

1. Crabtree, R. H. *The Organometallic Chemistry of the Transition Metals*, Wiley, 1998
2. Gupta, B. D.; Elias, A. J. Basic Organometallic Chemistry: Concepts, Syntheses and Applications Paperback, Universities Press; 2nd Edition (May 30, 2013).

Reference Books

1. Collman J. P.; Finke R. G.; Norton J. R. *Principles & Applications of Organo-transition Metal Chemistry*, University Science Books
2. Bhaduri S.; Mukesh, D. Homogeneous Catalysis: Mechanisms and Industrial Applications

Preparatory Course Material

1. Maiti, D. *Organometallic Chemistry*, NPTEL Course Material, Indian Institute of Technology Bombay, https://www.youtube.com/watch?v=ITfwjQemwMg&list=PLj_Alq7xw30l8iUgacWidP_83A0rZqlBR&index=1

Title	**Numerical Methods and Group Theory**	Number	CY515
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	M.Sc. (CY) Program	Type	Elective
Pre-requisite			

Objectives

The instructor will:

1. Basic mathematics and numerical techniques required for Chemistry students
2. Knowledge on error analysis to be used for laboratory courses
3. Provide the fundamentals of group theory to understand structure, chemical bonding and spectroscopy

Learning Outcomes

The students are expected to:

1. Ability to analyze data and perform error analysis on the data
2. Ability to understand and appreciate the mathematical and group theoretical concepts behind chemical theories

Contents

Mathematical Concepts: Vectors and Vector spaces, Operators, Orthogonal and Unitary matrices, Diagonalization, Matrix eigenvalue problems, Systems of linear algebraic equations, Determinants, Ordinary and partial differential equations, Fourier and Laplace transformation (15 lectures)
Numerical Methods: Errors in Data, Absolute and relative errors, Distribution of Errors, Central Limit Theorem, Linear regression and correlation, Interpolation, Roots of Equations, Algorithms for Matrix (15 Lectures)
Group Theory: Symmetry elements and Point Groups, Group postulates and definitions, Group multiplication tables, Subgroups and cosets, Symmetry classes and conjugates, Reducible and irreducible representations, Representations and character tables, Group theory and quantum mechanics, Group theory and chemical bonding, Applications of group theory to structures and spectroscopy, Group theory and crystal symmetry (12 Lectures)

Text Books

1. Kreyszig, E., (2011) *Advanced Engineering Mathematics*, 9th Ed., Wiley
2. Cotton, F. A., (2008) *Chemical Applications of Group Theory*, 3rd Ed., Wiley India

Reference Books:

1. Louis, L., (1991) *A Practical Guide to Data Analysis for Physical Science students*, Cambridge University Press
2. Louis, L., (2005) *Mathematics for Science Students*, Cambridge University Press
3. Arfken, W. and Harris, P. (2012) *Mathematical Methods for Physicists*, 7th Ed., Elsevier
4. Bishop, D. M., (1993), *Group Theory and Chemistry,* 2nd Ed., Dover Publications, New York

Preparatory Course Material:

1. Iyengar, S. R. K., *Numerical Methods and Computation,* NPTEL course material, Department of Mathematics, IIT Delhi
https://www.youtube.com/watch?v=88ys5ZIolSg&list=PL6E313980EF23CA6E
2. Chandra, M., Chemical Applications of Symmetry and Group Theory, NPTEL course material, Department of Chemistry, IIT Kanpur
https://www.youtube.com/watch?v=Av9f25sqLG0&list=PLj_Alq7xw30knZPTpa9whzqiSn_RZHGWP

Title	**Chemical Binding**	Number	CY524
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	M.Sc./Ph.D (Chemistry)	Type	Elective
Pre-requisite	CY 514 (Quantum Chemistry and Spectroscopy)		

Objectives

The Instructor will:

1. Provide high level understanding of a chemical bond using quantum mechanics.
2. Describe knowledge of modern techniques in quantum chemistry.

Learning Outcomes

The students are expected to:

1. Use modern quantum chemistry techniques to solve fundamental problems related to basic chemistry.
2. Understand a chemical bond.

Contents

Electronic structure: Variation theory, perturbation theory, electron spin, He atom, Pauli exclusion principle, Slater determinant (13 lectures)
Electronic structure of diatomic molecules: Born Oppenheimer approximation, Atomic units, H_2^+ ion, H_2 molecule, VB theory, MO theory, Semi-empirical methods (13 lectures)
Wave function based theory: Hartree-Fock theory, Electron correlation, Self-consistent field wave function, Moller-Plesset theory, Coupled cluster formulation (12 lectures)
Density functional theory (DFT): Principles of density functional theory, commercial functionals and applications (4 lectures)

Textbook

1. Levine, I. N., (2000) *Quantum Chemistry*, Pearson education.
2. Lowe, J. P., (1995) *Elementary Quantum Chemistry*, Academic Press.

Reference Books

1. Szabo, A. and Ostlund, N. S., (1996) *Modern Quantum Chemistry*, Dover.

Preparatory Course Material

K. Mangala Sunder, Introduction to Chemistry & Quantum Chemical Methods, NPTEL course material, Department of Chemistry, IIT Madras, http://nptel.iitm.ac.in

Title	**Principles of Nuclear Magnetic Resonance**	Number	CY6XX
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	M.Sc./PhD (CY) Program	Type	Elective
Prerequisite	CY211		

Objectives

The Instructor will:

1. Introduction to Nuclear Magnetic Resonance (NMR) Spectroscopy with an emphasis on the basic principle along with instrumentation and application.
2. Enable students to understand the design of NMR experiments and analyze NMR spectrum to extract information of interest.
3. Introduce to NMR experiments by giving hands on experience on the instrument available in the institute.

Learning Outcomes

The students are expected to:

1. Understand the theoretical background of solution state NMR.
2. Apply NMR experimental methods as an analytical tool in chemistry, biology, material science, medicine for structure and dynamic studies of molecules.
3. Understand instrumentation of NMR spectrometer available in the institute.

Contents

Introduction to NMR: Spin density operator, concept of density matrix, Liouville-Von-Neuman equation, the nuclear spin Hamiltonian- gyromagnetic ratio –energy level Diagrams-Zeeman Splitting. (12 lectures)

Introduction to NMR parameters: Chemical shifts and couplings, longitudinal and transverse relaxation process – Redfield relaxation theory – paramagnetic relaxation, correlation times and relaxation times. (10 lectures)

Introduction to 1D Fourier Transform spectroscopy: Bloch equation in the rotating frame – pulse sequence design – 1D 1H and 13C NMR for structure elucidation – measurement of relaxation rates, Nuclear Overhauser effect, effect of chemical exchange. (10 lectures)

Introduction to 2D NMR, correlation spectroscopy: common pulse sequences –homo and hetero nuclear correlation spectroscopy –examples of COSY, TOCSY and NOESY – Application –chemical structure –biological processes – molecular dynamics etc. aboratory demonstration of standard NMR experiments. (10 lectures)

Textbook

1. Farrar, T.C. and Becker, E.D., (1971), *Pulse and Fourier Transform NMR*, 1st Edition, Academic Press
2. Gunther, H., (1995), *NMR Spectroscopy*, 2nd Edition, Wiley
3. Derome, A. E., (1987), *Modern NMR Techniques for Chemistry Research*, 1st Edition, Pergamon Press

Reference Books

1. Ernst, R. R., Bodenhausen, G. and Wokaun, A., (1987), *Principles of Nuclear Magnetic Resonance in One and Two Dimension*, 2nd Edition, Clarendon Press
2. Claridge, T. D. W., (1999), High Resolution NMR Techniques in Organic Chemistry, 1st Edition, Elsevier

Preparatory Course Material

1. Atreya, H. S., *Principles and Applications of NMR Spectroscopy,* NPTEL Course Material, NMR Research Center, Indian Institute of Science, Bangalore, https://onlinecourses.nptel.ac.in/noc18_ge07

Title	**Quantum Information**	Number	CY652
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	M.Sc. (CY) Program	Type	Elective
Prerequisite	MA111		

Objectives

The Instructor will:

1. Provide fundamentals of quantum information and computation
2. Impart the knowledge of modeling efficiencies of a protocol in real experimental conditions

Learning Outcomes

The students are expected to:

1. Use the concepts taught in class to various aspects of quantum information, communication and cryptography
2. Understand and appreciate the technological evolution at theoretical and experimental front in QIC

Contents

Basics of quantum information: Review of linear algebra and basic laws of quantum mechanics, concept of bits and qubits, quantum gates, quantum parallelism, quantum algorithms, density operators and its applications (10 Lectures)

Quantum entanglement and nonlocality: Classical and quantum correlations, separability criterion, separable and entangled states, measures of two-qubit and multiqubit entanglement, Bell-type inequalities, discord (12 Lectures)

Quantum Noise: Classical and Markov Processes, Quantum Operations, Examples of Quantum Noise and Quantum Operations, Applications of Quantum Operations, Limitations of the Quantum Operations Formalism (6 Lectures)

Applications: Cryptography, quantum teleportation, dense coding, entanglement swapping, secret sharing, quantum games (10 Lectures))

Effects of noise on quantum information and computation (4 Lectures)

Textbooks

1. Nielsen, M. A. and Chuang, I. L., (2000) *Quantum Computation and Quantum Information*, 10th edition, Cambridge University Press.
2. Vedral, V., (2006) *Introduction to Quantum Information Science,* 1st edition, Oxford University Press

Reference Books

1. Griffiths, D. J., (2006) *Introduction to Quantum Mechanics*, 2nd edition, Pearson Prentice Hall.
2. Bouwmeester, D., Ekert, A. and Zeilinger, A., (2000) *The Physics of Quantum Information*, 2nd edition, Springer.
3. Bellac, M. L., (2006) *A Short Introduction to Quantum Information and Quantum Computation*, 1st edition, Cambridge University Press.

Preparatory Course Material

1. Goswami, D., *Quantum Computing*, *Mathematics for Chemistry,* NPTEL Course Material, Department of Chemistry, Indian Institute of Technology Kanpur https://onlinecourses.nptel.ac.in/noc18_cy07/preview

Title	**Molecular Dynamics Simulations**	Number	CY665
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	M.Sc./PhD (CY) Program	Type	Compulsory
Prerequisite			

Objectives

The Instructor will:

1. Provide high level understanding of the connection between dynamics of molecules and their macroscopic properties
2. Describe knowledge of modern techniques in molecular simulations using high speed computers

Learning Outcomes

The students are expected to:

1. Use modern simulation techniques to solve fundamental problems related to interdisciplinary areas of Physics, Chemistry and Biology
2. Find explanations for phenomena related to soft condensed matter

Contents

Basics of Molecular Dynamics: Theoretical foundation of classical statistical mechanics, Boltzmann's relation, harmonic oscillator and harmonic baths, introduction to molecular dynamics, Algorithms for equations of motions (10 lectures),
(few lectures overlap with "Computational Material Science" offered by Physics department)
Various ensembles: Purpose of ensembles in simulations, canonical ensembles, isobaric ensembles, grand canonical ensembles, applications of ensembles, thermostat, Barostat (10 lectures)
Advance Techniques: Free energy perturbation theory, Thermodynamic Integration, Jarzynski's equality, Umbrella Sampling (10 lectures)
Applications: How to set up Membrane system, protein and small biological molecules (10 lectures)

Textbooks

1. D. Frenkel and B. Smith, (2002), *Understanding Molecular Dynamics Simulations*,1st Edition, Academic Press
2. Mark Tuckermann, (2010), *Statistical Mechanics and Molecular Simulations*, 1st Edition, Oxford University

Self Learning Material

1. M. P. Allen and T. J. Tildesley., (1993), *Computer Simulations of liquids*, 1st Edition, Oxford Science Publications

Preparatory Course Material

1. Banerjee, T. *Molecular simulations*, NPTEL Course Material, Department of Chemical Engineering, Indian Institute of Technology Guwahati, http://nptel.ac.in/courses/103103036/
2. Tembe, B.L., *Computational Chemistry and Classical Molecular Dynamics*, NPTEL Course Material, Department of Chemistry, Indian Institute of Technology Bombay, https://onlinecourses.nptel.ac.in/noc18_cy13

Course Title	**Solid State NMR Methods for Materials**	Number	CY7XX
Department	Chemistry	L-T-P [C]	3-0-0 [3]
Offered for	MSc./PhD (CY) Program	Type	Elective
Prerequisite			

Objectives

The instructor will:

1. Introduction to essential techniques of solid state NMR
2. Introduction to various spin interactions important in solid state e.g., chemical shift anisotropy, dipolar coupling etc.
3. To enable students to analyze NMR spectrum to extract information on solid state structure and dynamics.

Learning Outcomes

The students are expected to:

1. Have basic understanding of the theoretical background of solid state NMR.
2. Application of solid state NMR in the field of materials relevant in medicine, renewable energy, polymers etc.
3. Understanding of various solid state methods that can be applied to characterize materials of interest.

Contents

Introduction to various nuclear spins other than 1H relevant for solid state materials: quadrupolar nuclei, concept of chemical shift anisotropy (CSA), scalar coupling, dipolar coupling and quadrupolar interactions, relation between shielding tensor and electronic structure, powder averaging. (8 lectures)

Introduction to nuclear spin Hamiltonian relevant in solid state: cross polarization, isotropic mixing Hamiltonian, solid state echo sequence, Homo and heteronuclear decoupling, concept of spin diffusion and polarization transfer, concept of Nuclear Quadrupole Resonance (NQR) (10 lectures)

Introduction to NMR techniques: powder line shape, determination of anisotropy, Magic Angle Spinning (MAS), generation of spinning sideband patterns, sideband modulation, molecular structure and dynamics determination by probing ssb manifolds, Techniques for measuring CSA and orientation of shielding tensor, measurement of homo and heteronuclear dipolar coupling, correlation experiments. (10 lectures)

Introduction to molecular dynamics: powder line shape analysis-relaxation time studies-2D rotor synchronization and Exchange Spectroscopy (EXSY). (10 lectures)

Application of solid state NMR: in polymers, nanomaterials, drugs, narcotics, explosives etc., recent advances in 1D solid state methods for dynamics, application of NQR. (4 lectures)

Text Books

1. Duer, J. M., (2005), *Introduction to Solid State NMR*, Wiley.

Reference Books

1. Ernst, R. R., Bodenhausen, G., Wokaun, A., (1987), *Principles of Nuclear Magnetic Resonance in One and Two Dimension*, Clarendon Press, Oxford.
2. Bakhmutov, V. I., (2011), *Solid-State NMR in Materials Science- Principles and Applications*, CRC Press.

Preparatory Course Material

1. Atreya, H. S., *Principles and Application of NMR spectroscopy*, NMR Research Center, IISC Bangalore, https://onlinecourses.nptel.ac.in/noc18_ge07/preview
2. Molugu, T. R., Lee, S., Brown, M. F., Concepts and Methods of Solid State NMR Spectroscopy Applied to Biomembranes, 2017, Chem. Rev., 117, 12087-12132
3. Dybowski, C., Bai, S., Solid State NMR Spectroscopy, 2008, Anal. Chem., 80, 4295-4300.

Title	**Quantum Computing**	Number	CY751
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	Ph.D. (CY) Program	Type	Elective
Prerequisite	MA111/CY514/PH513		

Objectives

The Instructor will:

1. Impart mathematical framework of Quantum Computation to students familiar with basic concepts of quantum mechanics and quantum information
2. Discuss advanced topics and State-of-the-Art research in quantum information and computation (QIC)

Learning Outcomes

The students are expected to:

1. Use the concepts taught in class to various aspects of quantum information, communication and cryptography
2. Understand and appreciate the technological evolution at theoretical and experimental front in QIC

Contents

Mathematical Preliminaries: Quantum Mechanics, Matrix representations of quantum states and operators, Cauchy-Schwartz and Triangle Inequalities, Classical and Quantum Correlations (6 Lectures)
Notions of Quantum Information: Classical and Quantum state Registers, Pure and Mixed states, Reduction and Purification of states, Quantum Channels, Completely Positive and trace Preserving Maps (6 Lectures)
Entropy: Quantitative bounds on Shannon and relative Entropy, Von-Neumann and quantum relative entropy, Klein's inequality, Concavity and subadditivity of von Neumann entropy, Strong subadditivity of von Neumann entropy, Accessible Information, Holevo information (8 Lectures)
Entanglement and Nonlocality: Separability Criteria, Classical, Separable and Entangled states, Local Operations and Classical Communications, Distillable entanglement and entanglement cost, Bound entanglement, Bell's Inequality and Nonlocality, Nonlocality in multiqubit Systems, Entanglement Measures (12 Lectures)
Quantum Error Correction: Bit flip and phase flip codes, Quantum Hamming Bound, Calderbank-Shor-Steane codes, Gottesman-Knil theorem, Fault-tolerant quantum computation, quantum algorithms and cryptography (10 Lectures)

Textbooks

1. Nielsen, M. A. and Chuang, I. L., *Quantum Computation and Quantum Information*, Cambridge University Press, 2000
2. Vedral, V., *Introduction to Quantum Information Science,* Oxford University Press, 2006

Reference Books

1. Griffiths, D. J., *Introduction to Quantum Mechanics*, Pearson Prentice Hall, 2006
2. Bouwmeester, D., Ekert, A. and Zeilinger, A., *The Physics of Quantum Information*, Springer, 2000
3. Bellac, M. L., *A Short Introduction to Quantum Information and Quantum Computation*, Cambridge University Press, 2006

Preparatory Course Material

1.Goswami, D., *Quantum Computing*, *Mathematics for Chemistry,* NPTEL Course Material,

Department of Chemistry, Indian Institute of Technology Kanpur
https://onlinecourses.nptel.ac.in/noc18_cy07/preview

Title	**Group Theory and Molecular Spectroscopy**	Number	CY6xx
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	MSc./Ph.D. (CY) Program	Type	Elective
Prerequisite			

Objectives

The Instructor will:

1. Provide basic and advanced group theoretical concepts and their applications in bonding, spectroscopy, and solid state chemistry.

Learning Outcomes

The students are expected to:

1. Analyze and understand the concept of point group and symmetry associated with molecular frameworks
2. Apply the knowledge of group theory to understand bonding, and structure in chemical species.

Contents

Introduction: The nature of the problem, symmetry operations, elements and operators, groups and group theory- general definitions, defining, deriving and recognizing point groups, subgroups and cosets, classes, group multiplication table (10 Lectures)
Theory of group representations: The great orthogonality theorem, character of a representation, reducible and irreducible representations, construction of character tables and physical interpretation, application of representation theory in quantum mechanics, direct-product groups (10 Lectures)
Applications to Chemical Bonding and spectroscopy: Molecular orbitals, applications to valence bond theory and molecular orbital theory, bonding in homonuclear diatomic molecules of transition metal, molecular orbitals in complex compounds, Huckel molecular orbital theory, application of group theory to UV-Visible, IR and Raman spectroscopy (14 Lectures)
Group theory and crystal symmetry: Crystal systems and classes, translational and space groups, symmorphic and nonsymmorphic space groups, applications of space group, factor group (8 Lectures)

Textbooks

1. Cotton, F. A., (1990) Chemical Applications of Group Theory, 3rd edition Wiley-Interscience
2. Vincent, A., (2013) *Molecular Symmetry and Group Theory: A Programmed Introduction to Chemical Applications*, 2nd Edition Wiley

Reference Books

1. Engel, T. and Reid, P., (2012), *Quantum Chemistry and Spectroscopy*, 3rd Edition, Pearson

Preparatory Course Material

1.Chandra, M., *Chemical Applications of Symmetry and Group theory*, NPTEL Course Material, Department of Chemistry, Indian Institute of Technology Kanpur, https://onlinecourses.nptel.ac.in/noc18_ch02/preview

Title	**Modern Electronic Structure Theory**	Number	CY6XX
Department	Chemistry	L-T-P [C]	3–0–3 [4]
Offered for	M.Sc./PhD (CY) Program	Type	Elective
Prerequisite	CY 514 (Quantum Chemistry and Spectroscopy)		

Objectives

The Instructor will:

1. Provide knowledge of modern electronic structure theories and basic computational chemistry techniques and tools to carry out electronic structure calculations and interpret experimental spectra

Learning Outcomes

The students are expected to:

1. Carry out electronic structure calculations and interpret experimental spectra
2. Write simple computer programs to carry out calculations

Contents

Review of basics: Linear algebra, numerical techniques, postulates of quantum mechanics, Born-Oppenheimer approximation, concept of potential energy surface, variational and perturbation approaches (14 lectures)
Electronic structure theories: Hartree-Fock (HF) and post-HF theories, Moller-Plesset theory, density functional theory, coupled cluster theory, electron correlation, configuration interaction, excited states, time dependent density functional theory (14 lectures)
Techniques: Energy minimization, vibrational frequency analysis, symmetry analysis, zero point energy calculation, intrinsic reaction coordinate, distinguishing stationary points, atomic charges, Mulliken analysis (14 lectures)

Laboratory Experiments

Electronic structure calculations; Geometry optimization; simple Fortran programming; finding intrinsic reaction coordinates; computing potential and free energy profiles

Textbook

1. Levine, I. N., (2016), *Quantum Chemistry,* 7th Edition, Pearson Education
2. McQuarrie, D. A., (2016), *Quantum Chemistry,* 2nd Edition, Viva Books
3. Szabo, A., (1996), *Modern Quantum Chemistry,* Dover Publications

Reference Books

1. Jensen, F., (2017), *Introduction to Computational Chemistry,* 3rd Edition, Wiley-Blackwell
2. Cramer, C. J., (2004), *Essentials of Computational Chemistry*, 2nd Edition, Wiley-Blackwell

Self Learning Course Material

1. Simons, J.: https://www.youtube.com/watch?v=Z5cq7JpsG8I

Title	**Chemical Reaction Dynamics**	Number	CY764
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	M.Sc./PhD (CY) Program	Type	Elective
Prerequisite	CY 514 (Quantum Chemistry and Spectroscopy)		

Objectives

The Instructor will:

1. Provide introduction to reaction dynamics in the gas phase and many advanced concepts in scattering theory.
2. Compare experimental data with dynamics simulations.

Learning Outcomes

The students are expected to:

1. Interpret experimental data in terms of classical and quantum scattering theory
2. Design and perform advanced dynamics simulations.

Contents

Reactive collisions: Fundamentals, Potential energy surfaces, Crossed molecular beams, state-to-state cross sections, Classical and quantum scattering process (15 lectures)
Rate theories: Kinetic theory of gases, Transition state theory (TST), Rice-Ramsperger-Kassel-Marcus (RRKM) theory, Microcanonical and thermal rate constants
Gas phase dynamics: Photodissociation, energy transfer dynamics, intramolecular vibrational energy flow, mode selective chemistry with Lasers (20 lectures)
Condensed phase dynamics: Solvation, Diffusion, Kramer-Grote-Hynes model, Correlation functions (7 lectures)

Textbooks

1. R. D. Levine, (2009) *Molecular Reaction Dynamics,* Reprint Edition, Cambridge University Press, USA.

Reference Books

1. T. Baer and W. L. Hase, (1996), *Unimolecular Reaction Dynamics: Theory and Experiments,* Oxford University Press, USA
2. A. Nitzan, (2006), *Chemical Dynamics in Condensed Phases,* Oxford University Press, USA

Preparatory Course Material

1. Halder, M., *Reaction Dynamics*, NPTEL lectures, Department of Chemistry, Indian Institute of Technology, Kharagpur, http://nptel.ac.in/courses/104105041/31

Title	**Biophysical Techniques: Theory and Applications**	Number	CY5XX
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	M.Sc/PhD Program, B.Tech	Type	Elective
Prerequisite			

Objectives

The Instructor will:

1. Introduce basic knowledge of a few biophysical methods and their application in the interdisciplinary area of chemistry and biology.
2. To have a greater understanding of the underlying theory of these methods and their practical applications in the laboratories.

Learning Outcomes

The students are expected to:

1. Understand the underlying principle of different biophysical methods.
2. To be able to use important biophysical methods to decipher problems relevant to biology.
3. Better understand the structure-function activity of biomolecules.

Course Content

Spectroscopic methods: Concepts of spectral transition and analysis of spectrum, Application of UV-VIS spectroscopy in protein folding kinetics, Advance topics in fluorescence such as anisotropy, resonance energy transfer and real time fluorescence; principle of Circular dichroism, optical rotatory dispersion methods and applications, Principle of Surface Plasmon Resonance spectroscopy, SPR optical phenomenon, application of SPR in ligand-protein interaction. (15 lectures)
Magnetic Resonance based methods: Principles of NMR and EPR, Concept of relaxation and polarization transfer, application of 1D and 2D NMR methods in biomolecules, EPR transitions, identification of metal centers in biomolecules, spin labelling and motions of side chains. (15 lectures)
Calorimetric techniques: Principles and applications of Isothermal Titration Calorimetry, Differential Scanning Calorimetry, applications in biomolecules. (7 lectures)
Centrifugation Techniques: Concepts and fundamentals of centrifugation. Ultracentrifugation techniques in biology. (5 lectures)

Textbook

1. Cox, M.M, Nelson, D.L., Lehninger (2009) *Principles of Biochemistry*, 6th Edition, W.H. Freeman & Co,
2. Gunther, H., (1995), *NMR Spectroscopy*, 2nd Edition, Wiley
3. *Circular Dichroism – Principles and Application*, (2000) Edited by Brova, N., Nakanishi, K., Woody, R. W., 2nd Ed., Wiley.

Reference Books

1. Claridge, T. D. W., (1999), High Resolution NMR Techniques in Organic Chemistry, 1st Edition, Elsevier
2. Stryer, L., Berg, J.M., Tymoczko, J.L., (2012) *Biochemistry*, W.H.Freeman & Co Ltd
3. Lakowicz, J. R., (2006), *Principles of Fluorescence Spectroscopy*, 3rd Edition, Springer, New York
4. Biophysical approaches determining ligand binding to biomolecular targets (2011), Edited by Podjarny, A., Dejaegere, A., Keiffer, B., RSC Publishing

Preparatory Course Material

1. NPTEL lectures: https://onlinecourses.nptel.ac.in/noc19_cy07/preview
2. Sharma, K. A., Analytical Technologies in Biotechnology, Dept. of Biotechnology, IIT Roorkee, https://onlinecourses.nptel.ac.in/noc19_cy07/preview

Course Title	**Stochastic Problems in Biophysics**	Number	CY758
Department	Chemistry	L-T-P [C]	3-0-0 [3]
Offered for	PhD (CY) Program	Type	Elective
Pre-requisite			

Objectives

The instructor will:

1. To understand applications of fundamental probability methods to wide variety of problems related to biophysics.
2. To show the mathematical literature on this subject
3. To understand non-equilibrium statistical mechanics

Learning Outcomes

The students are expected to:

1. Ability to translate complex phenomena into simple models
2. Ability to derive mathematical models for problems related to biophysics

Course Content

1. *Introduction:* Historical examples, Joint and conditional Probabilities, Correlation functions and Cumulants, Gaussian and Poissonian Probability Distributions (14 lectures)
2. *Markov Processes*: Chapman-Kolmogorov Equation, Examples of Markov Processes (10 lectures)
3. *Brownian Motion:* Basic assumptions, Langevin Equation, Fokker-Planck Equation, Master Equations and Jump Processes, Linear Response Theory (18 lectures)

Text Books

1. Landau and Lifshitz, *Statistical Physics*, Elsevier, 2005
2. David Chandler, *Introduction to Modern Statistical Mechanics*, Oxford University Press, 1987

Self Learning Materials

1. C. W. Gardiner, *Handbook of Stochastic Methods for Physics, Chemistry and Natural Sciences*, Springer-Verlag, 1983
2. Edited and Introduced by John Stachel, *Einstein's Miraculous Year*, Princeton University Press, 1998.
3. S. Chandrashekhar, Reviews of Modern Physics, vol 15, No 1, APS

Preparatory Course Material

Prof. V. Balakrishnan, IIT Madras: https://www.youtube.com/watch?v=qNmB1qNjZ0k

Course Title	**Polymer Dynamics**	Course No.	CY760
Department	Chemistry	L-T-P[C]	3-0-0 [3]
Offered for	PhD (CY) Program	Type	Elective
Pre-requisite			

Objectives
The instructor will:
To understand basic principles and theory of modern macromolecules
To understand the analogy to other branches of science at a more fundamental level

Learning Outcomes
The students are expected to:
1. Ability to realize that polymers are essential ingredients in biological machinery
2. Ability to do advanced calculations more modestly

Course Content
Ideal Chain : Freely joint chain, Flexibility of a polymer chain, Gaussian Chain, Ideal chain as a random walk, Ideal polymer by an external force, Flory Calculation (12 lectures)
Polymer chains with volume interactions and Melts : Models with volume interactions, ideal melts, chains in solvents (10 lectures)
Dynamics: Rouse model, Zimm Model, Real polymer coil, Reptation model (10 lectures)
Biopolymers: Properties, Primary structure, Secondary structure, Helix-coil transition (10 lectures)

Text Books
1. M. Doi and S. F. Edwards, *The Theory of Polymer Dynamics*, Oxford Science Publications, 1990.

Self Learning Materials
1. Alexander Yu. Grosberg and Alexei R. Khokhlov, *Statistical Physics of Macromolecules*, AIP Press, 1994
2. Pierre-Gilles de Gennes, *Scaling Concepts in Polymer Physics*, Cornell University Press, 1979

Online course material
1. George Phillies lectures a series of graduate classes, based on his book "Phenomenology of Polymer Solution Dynamics" Cambridge University Press, 2011.
2. https://www.youtube.com/watch?v=mVzrYKkeJzE

Course Title	**Statistical Mechanics and Molecular Simulations**	Course No.	CY758
Department	Chemistry	L-T-P [C]	3-0-0 [3]
Offered for	PhD (CY) Program	Type	Elective
Pre-requisite			

Objectives

The instructor will:

1. To understand the complex soft matter system that bridges the traditional disciplines of physics, chemistry and biology using modern theoretical methodology and high-speed computers.
2. To explore the connections between basic statistical mechanical theories and real world applications in studying physical, chemical and biological phenomena.

Learning Outcomes

The students are expected to:

1. Understanding basic principles of Statistical Mechanics and Molecular Dynamics Simulations.
2. Mathematical formalism associated with theory and techniques of molecular modelling.
3. Few real world applications to understand the connections between microscopic and macroscopic world.

Course Content

Statistical basis of thermodynamics: Introduction to Statistical Methods, Micro and Macro states, Ensemble theory (micro-canonical, canonical, isobaric, grand-canonical), Mathematical techniques (5 lectures)

Classical Statistical Mechanics: Partition functions, Thermodynamic functions, Phase space and Liouville equation, Distribution functions, Kirkwood integrals (10 lectures).

(Module 3 of ``Statistical Physics" by Physics department) *Fluctuations:* Thermodynamic fluctuations, Spatial correlations in a fluid, Einstein-Smoluchowski theory of Brownian motion, Langevin theory,Fokker-Planck equation, Fluctuation-dissipation theory, Onsager relations (12 lectures)

Introduction to Molecular Modeling: Algorithms, Periodic boundary conditions, Interaction functions and force fields, Electrostatics, Molecular dynamics in various ensembles (10 lectures)

Applications: Brownian dynamics simulations, Biological applications for proteins and membranes (5 lectures)

Text Books

1. Mark E Tuckerman, *Statistical Mechanics and Molecular Simulations*, Oxford University, 2010
2. David Chandler, Introduction to Modern Statistical Mechanics, Oxford University Press, 1987

Self Study Material

1. M. P. Allen and T J Tildesley, *Computer Simulations of Liquids*, Oxford Science Publications, 1993
2. D. A. Mcquarrie, *Statistical Mechanics*, University Science Books, 2000
3. D. Frenkel and B. Smit, *Understanding Molecular Dynamics Simulations*, Academic press, 2002
4. Andrew R Leach, *Molecular Modelling: Principles and applications*, Prentice Hall, 2010
5. R K Pathria, Paul D. Beale, *Statistical Mechanics*, Elsevier, 2011

Preparatory Course Material

1. https://ocw.mit.edu/courses/mechanical-engineering/2-57-nano-to-macro-transport-processes-spring-2012/

Course Title	**Advanced Electrochemistry and Applications**	Number	CY6xx
Department	Chemistry	L-T-P [C]	3–0–0 [3]
Offered for	M.Sc/PhD Program	Type	Elective
Pre-requisite			

Objectives

The instructor will

1. Provide an introductory but thorough background in electrochemistry.
2. Provide fundamentals of electrochemical systems, electroanalytical techniques and advanced applications.

Learning Outcomes

The students are expected to:

1. describe the difference between equilibrium properties and properties of electrochemical systems and apply electrochemical methods for required information.
2. explain the functioning of electrochemical devices as well as the commonly employed underlying electrochemical reactions

Contents

Introduction to Electrochemistry: Nernst equation, electrode kinetics, dynamic electrochemistry, the Butler-Volmer and Tafel equations. Overpotentials. Kinetically and mass transport controlled electrochemical processes. Mass transport by migration, convection and diffusion. Conductivity. (Lectures 7)

Electrochemical Methods: Potentiostatic and galvanostatic electrochemical methods including chronoamperometry, coulometry, cyclic voltammetry, chronopotentiometry, ac impedance spectroscopy, spectroelectrochemistry and hydrodynamic methods.(Lectures 8)

Solid state electrochemistry. Ion conducting and electronically conducting polymers; The electrochemical double layer. (5 Lectures)

Surface confined electrochemical processes: The fundamentals of corrosion. Homogeneous and heterogeneous electrocatalysis (HER and OER). Electrochemical processes coupled to chemical steps. Nanostructured and surface modified electrodes. (8 Lectures)

Application: Introduction to batteries, fuel cells and electrochemical solar cells. (7 Lectures)

Electrochemical processes of particular relevance to energy conversion.(5 Lectures)

Text Books

D. I. Antropov, Theoretical Electrochemistry, Mir Publishers, 1972.

J. M. Bockris and A. K. N. Reddy, Modern Electrochemistry, Vol.1 and 2, Plenum Press, 1998.

Industrial Electrochemistry, 2nd ed, Pletcher, Derek/Walsh, Frank C., London: Chapman and Hall, 1990

Electrochemistry for Chemists, 2nd ed, Sawyer, Donald T./Sobkowiak, Andrej/Roberts, Julian L., New York: John Wiley, 1995

Reference Books

1. Transient Techniques in Electrochemistry, Macdonald, Digby D., New York: Plenum Press, 1977
2. Laboratory Techniques in Electroanalytical Chemistry, (2nd edition) by Peter Kissinger and William Heineman (Marcell Dekker) 1996

Preparatory Course Material

1. https://nptel.ac.in/courses/104106105/