CHEMICAL SCIENCES, Int MSc-Ph.D.

Programme Code: CHEM04

Programme Outcome:

- Foundation in the fundamentals of core chemical sciences fields including those in Analytical, Inorganic, Nuclear and Physical Chemistry.
- Skill development in critical thinking and problem solving applied to scientific problems.
- Development of skills to clearly communicate the results of scientific work in oral, written and electronic formats to both scientists and the public at large.
- Development of skill set necessary for starting a research career in chemical sciences and allied areas
- Appreciate the central role of chemistry in DAE programmers and apply these to take up research in key issues such energy, health and medicine

DETAILED COURSE STRUCTURE

Semester	Course No.	Course Name	Hours		Credits
			L	T	
Semester-I	CHE701	Physical Organic Chemistry	45	15	4
	CHE702	Molecular Quantum Mechanics	45	15	4
	CHE703	Chemistry of Main Group (s and p-block) Elements	45	15	4
	CHE741	Inorganic Chemistry Laboratory (6hr/week)		84 (P)	3
Semester-I	CHE704	Molecular Spectroscopy and Group theory	45	15	4
	CHE705	Coordination Chemistry	15	45	4
	CHE706	Advanced Organic Chemistry	15	45	4
	CHE742	Organic Chemistry Laboratory (6hr/week)		84 (P)	3
Semester-III	CHE801	Heterocyclic and Natural Product Chemistry	15	45	4
	CHE802	Organometallic Chemistry	15	45	4
	CHE***	Elective - I	15	45	4
	CHE841	Physical Chemistry Laboratory (6hr/week)		84 (P)	3
Semester-IV	CHE803	Applied Spectroscopy	45	15	4
	CHE842	Computational Chemistry Lab, 6hr/week		84(P)	3
	CHE***	Elective II	15	45	4
	CHE***	Elective III	15	45	4
	CHE843	Research Laboratory, 8hr/week contact hours	0, p/f*		

Semester	**Course Code**	**Courses Name**	Hour		**Credit**
			T	L	
Semester-V	CHE901	Specific-Research Works for M. Sc.	45	15	4
	CHE800	Research Methodology and Research and publication ethics (requirement for PhD program)	45	15	3
Semester-VI	CHE902	Specific-Research Works for M. Sc.		180(P)	6
* p/f: pass/fail course with 0 credit *** electives I-V have to be from the list of elective courses					

SYLLABUS FOR ELECTIVE COURSES

	Elective Course			
Course No.	Course Name	Hours		Credits
		L	T	
CHE901	Photochemistry	45	15	4
CHE902	Pharmaceutical Chemistry	45	15	4
CHE903	Classics in Molecules	45	15	4
CHE904	Molecular Modeling	45	15	4
CHE905	Solid State Chemistry	45	15	4
CHE906	Crystallography	45	15	4
CHE907	Principles of Drug Action	45	15	4
CHE908	Advanced Bio-inorganic Chemistry	45	15	4
CHE909	Nuclear Magnetic Resonance	45	15	4
CHE910	Advanced Functional Materials	45	15	4
CHE911	Supramolecular Chemistry	45	15	4
CHE912	Chemistry of Nanomaterials	45	15	4
CHE913	Advanced Bio-organic Chemistry	45	15	4
CHE914	Polymer Chemistry	45	15	4
CHE915	Molecular Reaction Dynamics	45	15	4
CHE916	Theory of Molecular Spectroscopy	45	15	4
CHE918	Catalysis: Reaction Mechanisms and Applications	45	15	4
CHE919	Advanced Main Group Chemistry	45	15	4
CHE920	Advanced Fluorescence Spectroscopy	45	15	4
CHE921	Bio macromolecules	45	15	4
CHE922	Advanced Heterocyclic Chemistry	45	15	4

CHE923	Statistical Mechanics	45	15	4
CHE924	Frontiers in Organic Synthesis	45	15	4

CORE COURSES COORDINATOR

Chief Coordinators: Dr. B. L. Bhargava (Email: convener_ugcsc@niser.ac.in) **&** Prof. V. Krishnan (Email: convener_pgcsc@niser.ac.in)

Core Course		
Course Name	**Coordinator Name**	**Email ID**
Physical Organic Chemistry	Prof. Prasenjit Mal	pmal@niser.ac.in
Molecular Quantum Mechanics	Prof. Himansu S. Biswal	himansu@niser.ac.in
Chemistry of Main Group (s and p-block) Elements	Prof. V. Krishnan	krishv@niser.ac.in
Inorganic Chemistry Laboratory (6hr/week)	Dr. Bidraha Bagh	bidraha@niser.ac.in
Molecular Spectroscopy and Group theory	Prof. Subhadip Ghosh	sghosh@niser.ac.in
Coordination Chemistry	Dr. Deepak Samanta	dsamanta@niser.ac.in
Advanced Organic Chemistry	Dr. Rajkumar Misra	rajkumarmisra@niser.ac.in
Organic Chemistry Laboratory (6hr/week)	Dr. S. Peruncheralathan	peru@niser.ac.in
Heterocyclic and Natural Product Chemistry	Prof. C. Gunanathan	gunanathan@niser.ac.in
Organometallic Chemistry	Prof. S. Nembenna	snembenna@niser.ac.in
Physical Chemistry Laboratory (6hr/week)	Prof. Himansu S. Biswal	himansu@niser.ac.in
Applied Spectroscopy	Dr. Bishnu P. Biswal	bp.biswal@niser.ac.in
Computational Chemistry Lab, 6hr/week	Prof. U. Lourderaj	u.lourderaj@niser.ac.in

ELECTIVE COURSES COORDINATOR

Elective Course		
Course Name	**Coordinator Name**	**Email ID**
Photochemistry	Dr S. Peruncheralathan	peru@niser.ac.in
Pharmaceutical Chemistry		
Classics in Molecules		
Molecular Modeling	Prof. U. Lourderaj	u.lourderaj@niser.ac.in
Solid State Chemistry	Prof. J. N. Behera	jnbehera@niser.ac.in
Crystallography		
Principles of Drug Action	Dr. S. Peruncheralathan	peru@niser.ac.in
Advanced Bio-inorganic Chemistry	Prof. Sanjib Kar	sanjib@niser.ac.in
Nuclear Magnetic Resonance	Dr. Arindam Ghosh	aringh@niser.ac.in
Advanced Functional Materials	Prof. Sudip Barman	sbarman@niser.ac.in
Supramolecular Chemistry	Dr. C. S. Purohit	purohit@niser.ac.in
Chemistry of Nanomaterials	Prof. Sudip Barman	sbarman@niser.ac.in
Advanced Bio-organic Chemistry	Dr. N. K. Sharma	nagendra@niser.ac.in
Polymer Chemistry	Prof. V. Krishnan	krishv@niser.ac.in
Molecular Reaction Dynamics	Prof. U. Lourderaj	u.lourderaj@niser.ac.in
Theory of Molecular Spectroscopy		
Catalysis: Reaction Mechanisms and Applications	Prof. C. Gunanathan	gunanathan@niser.ac.in
Advanced Main Group Chemistry	Prof. Sharanappa Nembenna	snembenna@niser.ac.in
Advanced Fluorescence Spectroscopy	Prof. Moloy Sarkar	msarkar@niser.ac.in
Biomacromolecules	Dr. C. S. Purohit	purohit@niser.ac.in

Advanced Heterocyclic Chemistry	Dr. N. K. Sharma	nagendra@niser.ac.in
Statistical Mechanics	Dr. B. L. Bhargava	bhargava@niser.ac.in
Frontiers in Organic Synthesis	Dr. S. Peruncheralathan	peru@niser.ac.in

1st YEAR, SEMESTER-I

CHE701: Physical Organic Chemistry (45L+15T Hours)

Coordinators: Prof. Prasenjit Mal
pmal@niser.ac.in

Course Details:

- **Stereoelectronic Effects**
  Anomeric & related effects; Acetals, Esters, Amides and related functions; Reactions at sp3, sp2, and sp Carbons; Examples in synthesis and biological processes; Felkin–Ahn Model, Houk Model, Cieplak Model, EFOE Model, and Cation-complexation model as applied to π–Facial Selectivity; Baldwin's Rule.

- **Pericyclic Reactions**
  The nature of pericyclic Reactions; The Woodward-Hoffmann Rules and Molecular Orbitals; Cycloaddition reactions; Electrocyclic Reactions; Sigmatropic Rearrangements- [1,2], [1,3], [1,5], [2,3] and [3,3]; Cheletropic Reactions; Cope Rearrangements; Claisen Rearrangements; Enantioselective Pericyclic Reactions.

- **Photochemistry**
  Electronic Configurations – Multiplicity, S0, S1, T1; Electronic Transitions – π to π*, n to π*; Selection Rules and Solvent Effect on π to π*, n to π* transitions; Photochemistry of Olefins, Dienes and Carbonyl Compounds; Chemistry of Vision.

- **Radical Reactions**
  Generation and Characterization of Free Radicals; Nucleophilic and Electrophilic Radicals; Substitution Reactions; Addition Reactions; Radical Coupling; Barton Reaction.

Course Outcomes:

- Understanding the Molecular Orbitals and Woodward-Hoffmann Rules. Application in stereoselective organic synthesis.
- Photoinduced chemical reactions.
- Radical initiated processes and radical intermediates in chemical reactions

References:

1. F. A. Carey, R. J. Sundberg "Advanced Organic Chemistry Part B: Structure and Mechanisms" 5th Edn., Springer, 2007.
2. R. Bruckner "Organic Mechanisms: Reactions, Stereochemistry and Synthesis" Springer, 2010.
3. J. Clayden, N. Greeves, S. Warren, P. Wothers "Organic Chemistry" Oxford University press, 2001.
4. M. B. Smith, J. March "March's Advanced Organic Chemistry" 6th Edition, Wiley-VCH, 2007.
5. E. V. Anslyn, D. A. Dougherty "Modern Physical Organic Chemistry" California University Science Books, 2006.
6. Fleming "Molecular Orbitals and Organic Chemical Reactions" Wiley-VCH, Student Edition, 2010.
7. M. Coxon, B. Halton "Organic photochemistry" Cambridge University Press, 1974.
8. H. Depuy and O. L. Chapman "Molecular Reactions and photochemistry", Prentice Hall of India, 1975.

CHE702: Molecular Quantum Mechanics (45L+15T Hours)

Coordinators: Prof. Himansu S. Biswal
himansu@niser.ac.in

Course Details:

- **Introduction to quantum mechanics**
  Postulates of quantum mechanics, de Broglie Hypothesis, Uncertainty Principle, The Time-Independent Schrödinger Equation, Interpretation of wave function, Probability density, Mathematical background – vectors, matrices, and operators.

- **Simple applications of quantum theory**
  Particle in a One-Dimensional Box, Particle in a Three-Dimensional Box, Degeneracy, One-Dimensional Harmonic Oscillator, Two-Particle Rigid Rotor, The Hydrogen Atom, Angular Momentum.

- **Approximation Methods**
  Vibrational and perturbation methods.

- **Atomic Structure**
  Electron Spin, Helium Atom and the Spin–Statistics Theorem, Total Orbital and Spin Angular Momenta, Many-Electron Atoms, Atomic Terms.

- **Molecular Electronic Structure**
  Born–Oppenheimer Approximation, Hydrogen Molecule Ion, Simple Molecular Orbital Method for Diatomic Molecules, Molecular Terms for diatomic, Valence-Bond Method. [8] Hückel Molecular Orbital theory and Introduction to Hartree method.

Course Outcomes:

- Basic understanding of the principles of quantum mechanics
- Knowledge of solutions to the Schrödinger equation for model systems
- Application of approximation methods in solving the Schrödinger equation
- Understanding of molecular orbital theory and valence bond theory

References:

1. N. Levine, Quantum Chemistry, Prentice-Hall of India, 2006.
2. P. W. Atkins and R. S. Friedmann, Molecular Quantum Mechanics, Oxford, 2008.
3. D. A. McQuarrie and J. D. Simon, Physical Chemistry – A Molecular Approach, Viva Books, New Delhi, 1998.

CHE703: Chemistry of Main Group (s and p-block) Elements (45L+15T Hours)

Coordinators: Prof. V. Krishnan
krishv@niser.ac.in

Course Details:

- **Chemistry of alkali and alkaline earth elements**
  Structure and bonding in alkali and alkaline earth metal Complexes-Alkali metal chemistry with carbon based ligands and Group 14 and 15 alkali metal bonded complexes. Low oxidation state with M-M bonded alkaline earth metal complexes; Synthesis and reactivity studies.

- **Chemistry of Boron, Aluminum and Silicon**
  Boranes, Carboranes and heterocarboranes, Multiple bonded main group compounds containing B-B double and triple bonds, Al-Al double bond and Si-Si double and triple bonds: Synthesis and reactivity studies.

- **Main group metal compounds in Homogenous Catalysis**
  Group 2 metal complexes in catalytic reactions such as hydroboration, hydrosilylation, hydroamination, dehydrocoupling, hydrogenation and hydrophosphination.

- Group 13 and 14 (B, Al, Si and Ge) based molecular compounds in homogenous catalysis.

Course Outcomes:

- Learn the basic concepts of early main group elements
- Study the structure and bonding aspects of unusual main group molecules
- Understanding the structure and bonding aspects of metal-metal single or multiple bonds of main group elements
- Knowledge of s- and p-block metal-based catalysts in organic transformations

Reference:

1. C. Elschenbroich Organometallics 93rd Edition Wiley-VCH, 1992
2. Alkaline earth metal compounds: Oddities and applications, Editor S Harder (topics in Organometallic Chemistry 45), 2015 4.
3. Comprehensive Organometallic Chemistry III: Editors in Chief Robert H Crabtree and D M P Mingos Vol. 2 Compounds of Groups 1-2 and 11-12 Volume Editor: Karsten Meyer, 2007
4. Comprehensive Organometallic Chemistry III: Editors in Chief Robert H Crabtree and D M P Mingos, Vol. 3 Compounds of Groups 13 and 15 Volume Editor: C E Housecraft, 200

CHE741: Inorganic Chemistry Laboratory (84P Hours)

Coordinators: Dr. Bidraha Bagh
bidraha@niser.ac.in

Course Details:

- A) Synthesis of Fe(salen)Cl complexes; B) Elucidation of Redox behavior of Fe(III) and C) Elucidation of magnetic properties. Chemistry of Natural Products
- Synthesis of meso tetratolul porphyrin from pyrrole and p-tolualdehyde and B) Synthesis and characterization of zinc-porphyrin (meso-tetratolyl porphyrin) complex.
- Separation of the chromium complexes by using ion exchange column.
- Preparation and determination of the effective magnetic moment and number of unpaired electrons in Mn(acac)3.
- Preparation and determination of the aquation rate of [Co(NH3)5Cl]Cl2.
- Friedel-Craft acylation of ferrocene.
- Synthesis and reactivities of organocobaloximes.
- Preparation of tris(acetylacetonato) iron(III).
- Preparation tris(ethylenediammine)cobalt(II) ion and its resolution into optical antipodes.
- Preparation of an iron (or nickel) nitrosyl complex.
- Preparation of boronic acid from Grignard reagents and trimethyl borate.
- Preparation of chiral salen based catalysts of Co, Cr derived from 3,5-di-tert butylsalicylaldehdye and trans-1,2-diaminocyclohexane.

Course Outcomes:

- Learn laboratory safety
- Learn synthesis, purification, extraction and recrystallization techniques along with various techniques for characterization viz. IR, UV-Vis Spectroscopy, CV (cyclic voltammetry), and magnetic susceptibilities.
- Learn preparation and use of ion exchange column which is used in pharmaceutical Industry.
- Familiarization with advanced techniques for syntheses and characterization of coordination compounds and organomatallic complexes including the use of standard Schlenk and vacuum line techniques.
- Crystallization, distillation and sublimation as purification methods will be practiced. • Able to clearly communicate the results of scientific work in oral, written and electronic formats to both scientists and the public at large

Reference:

1. Handbook of Preparative Inorganic Chemistry, Vol. i & ii (edited by G. Brauer), Academic Press, 1963.
2. Experimental Electrochemistry for Chemists, D. T. Sawyer and J. L. Roberts, Jr., John Wiley & Sons, New York, 1974.
3. Vogels Textbook of Quantitative Chemical analysis, G. H. Jeffery, J. Bessett, J. Medham and R. C. Denny, 5th Edn., ELBS, 1999.
4. J. D. Woollins, Inorganic Experiments, 2nd Ed, Wiley-VCH, Weinheim (2003).
5. M. A. Malati, Experimental Inorganic/Physical Chemistry: An Investigative, Integrated Approach to Practical Project Work, Horwood Publishing Ltd, England (1999).
6. J. Tanaka, S. L. Suib, Experimental Methods in Inorganic Chemistry, Prentice Hall, New Jersey (1999).

1st YEAR, SEMESTER-II

CHE704: Molecular Spectroscopy and Group Theory ((45L+15T Hours)

Coordinators: Prof. Subhadip Ghosh
sghosh@niser.ac.in

Course Details:

- **Group Theory**
  Symmetry elements, Symmetry operations, Point groups, Symmetry representations; Applications of symmetry to Molecular Orbital diagrams of simple molecules (examples: H2O, BeH2, BF3($\sigma + \pi$)); Definition of a group and basic theorems, Molecular symmetry groups and classes, Great Orthogonality Theorem; Matrix representation of groups, Irreducible representations and Character Tables, Symmetry properties of wave functions, Orbitals as basis sets for irreducible representations, Symmetry adapted linear combinations, Assignment of symmetry representations of d-orbitals for specific geometries.

- **Introduction to Spectroscopy**
  Interaction of light with matter, Transition moments and transition probabilities, Einstein's coefficients, Oscillator strength.

- **Diatomic Molecules**

  - **Electronic Spectra**
    Born–Oppenheimer approximation, Potential energy curves of diatomic molecules, Frank–Condon principle, Electronic transitions in homonuclear and heteronuclear diatomics.

  - **Microwave and Infrared Spectroscopy**
    Simple harmonic oscillator and Rigid Rotor Model, Rotational spectra of diatomic molecules, Stark effect, Vibrational spectra of diatomic molecules, Anharmonic correction, Selection rules, Fundamental and Overtone bands, Isotope effects, Vibrational Rotational coupling.

- **Diatomic Molecules**

  - **Electronic Spectra**
    Electronic structure, Electronic spectra of polyatomic molecules – linear conjugated molecules, Aromatic molecules, Transition metal compounds, Fluorescence, Phosphorescence, Internal conversion and Charge transfer.

  - **Rotational, Vibrational and Electronic Spectroscopy of polyatomic Molecules**
    Symmetric and asymmetric top molecules, Normal modes of vibration and their classification by group theory, Coupling between rotational and vibrational degrees of freedom. Symmetry and normal modes of vibration. Rovibrational spectra, Concept of anisotropic polarizability and Raman spectra.

Course Outcomes:

- Understand the fundamentals of Group Theory and apply it to molecular spectroscopy.
- Understand the link between molecular spectroscopy, symmetry and information content of molecular spectra.
- Understanding the formation of molecular orbitals.
- Calculate/predict energy levels and spectral features using symmetry as a simplification tool.
- Use symmetry arguments to possibly solve molecular Problems.
- Understand the fundamentals of rotational, vibrational and electronic spectroscopy.
- Calculation of some useful parameters from spectral data.

Reference:

1. Chemical Applications of Group Theory, F.A. Cotton, John Wiley, 3rd Edn., 2003.
2. Symmetry and Spectroscopy: An Introduction to Vibrational and Electronic Spectroscopy, D. C. Harris and M. D. Bertolucci, Dover, 1989.
3. Fundamentals of Molecular Spectroscopy, C. N. Banwell and E. M. McCash, Tata McGraw Hill, 1995.
4. Molecular Spectroscopy, G. M. Barrow, McGraw Hill, 1985.
5. Spectra of atoms and Molecules, P. F. Bernath, Oxford Univ. press, 2005.
6. Modern Spectroscopy, J. M. Hollas, John Wiley, 4th Edn., 2004.
7. Molecular Symmetry and Group Theory, R. L. Carter, John Wiley and Sons, 1998.

CHE705: Coordination Chemistry (45L+15T Hours)

Coordinators: Dr. Deepak Samanta
dsamanta@niser.ac.in

Course Details:

- **Theories of bonding**
  CFT including Jahn–Teller Effects of ligand field, Spectrochemical series, Enthalpies of hydration, Spinel structures. Shortcomings of CFT. MO theory of coordination complexes. Electronic Spectra of complexes including Orgel diagrams and Tanabe Sugano diagrams.

- **Magnetism**
  Introduction to Magnetism. Origin of diamagnetism. Para magnetism: Van Vleck formula and its approximated forms, Curie law. Magnetic susceptibility, Orbital quenching and spin-only moment; Magnetic exchange interactions in coordination compounds: Ferrimagnetism and Ant ferromagnetism; Bulk magnetic properties and ferromagnetism; Molecule-based magnetic materials: Organic magnets and single molecule magnets.

- **Mechanisms of reactions of transition metal complexes**
  Substitution (Kinetic effects: labile vs inert) and electron-transfer reactions (Outer-sphere, Self-exchange; Inner-sphere).

- **Bioinorganic Chemistry**
  Basic principles (why specific metal ions are present in certain proteins/enzymes): Heme proteins, types, structure and function (including mechanism of function): Hemoglobin, myoglobin, Cytochrome C, Cytochrome p450, Catalases, peroxidases. non-Heme proteins: Hemerythrin,

  Ribonucleotide reductase, Methanol monooxygenase (a) Iron-Sulfur proteins: Rubredoxin, Ferredoxin; (b) DNA / RNA: Ribozymes.

- **Transition metal based supramolecular structures**
  Ligand design and applications.

- **Mass Spectrometry**
  Basic concepts; Instrumentation, Fragmentation and rearrangements (including McLafferty rearrangement) of different classes of organic molecules; Isotope effects.

Course Outcomes:

- Importance of Crystal Field Theory and Molecular Orbital Theory with various inorganic complexes.
- Learn the concept of magnetism and also to know about single molecular magnet
- Understanding the inner and outer sphere reaction mechanisms.
- Role of metal ions in bioinorganic chemistry
- Understand the basic concepts of supramolecular chemistr

Reference:

1. Advanced inorganic Chemistry, F. A. Cotton, C. A. Murillo, and M. Bochmann, Wiley Interscience, 2001.
2. Inorganic Chemistry, D. F. Shriver and P. W. Atkins, Oxford University Press, 1999.
3. Supramolecular Chemistry: Concepts and Perspectives, J. M. Lehn, VCH, 1995.
4. Principles of Bioinorganic Chemistry, S. J. Lippard and J. M. Berg, Panima Publications, New Delhi, 1997.
5. Bioinorganic Chemistry; Inorganic Elements in the Chemistry of Life. Kaim, B. Schwederski Wiley, 1994.
6. Biological Inorganic Chemistry: Structure and Reactivity Harry B. Gray, E. I. Stiefel, J. S. Valentine, I. Bertini University Science Book; 2006.
7. Reaction Mechanism of Inorganic and Organometallic Systems, R. B. Jordan, 2nd Edn., Oxford University press, 1991.
8. Bioinorganic Chemistry, A. K. Das, Allied Books, Kolkata, 2004.
9. Molecular Symmetry and Group Theory: A programmed Introduction to Chemical Applications, A. Vincent, John Wiley, 2001.
10. Mechanism of Inorganic Reactions, F. Basolo and R. G. Pearson, 2nd Edn. Wiley, 1967.
11. Inorganic Reaction Mechanisms, M. L. Tobe and J. Burgess, 1st Edn., Wesley Longmans Ltd. 1999.
12. Inorganic Chemistry- Principles of Structure and Reactivity, J. E. Huheey, E. A. Keiter, R. L. Keiter and O. Medhi, Pearson Education, 2007.

CHE706: Advanced Organic Chemistry (45L+15T Hours)

Coordinators: Dr. Rajkumar Misra
rajkumarmisra@niser.ac.in

Course Details:

- Review of basic bonding concepts; Conformational analysis; Stereochemistry; Kinetics and Thermodynamics of Organic Reactions; Reaction Mechanisms and Conformational Effects on Reactivity; Oxidation Reactions; Reductions Reactions; Enolate Chemistry; Metalation Reactions; Key Ring Forming Reactions; Olefin Synthesis; Conjugate Additions; Synthetic analysis and Design; Total Synthesis of natural products; Asymmetric Synthesis; Combinatorial Chemistry.

Course Outcomes:

- Understanding of important organic transformations with advanced mechanisms
- Learning the recent advances in organic chemistry
- Enhanced ability to connect the learned topics with current research problem and envisage new research projects

Reference:

1. E. V. Anslyn, D. A. Dougherty, "Modern Physical Organic Chemistry" California University Science Books, 2006.
2. E. L. Eliel, S. H. Wilen, "Stereochemistry of Organic Compounds" Wiley-interscience, 1994.
3. R. Bruckner, "Organic Mechanisms: Reactions, Stereochemistry and Synthesis" Springer, 2010.
4. F. A. Carey, R. J. Sundberg, "Advanced Organic Chemistry Parts A & B: Structure and Mechanisms" 5th Edn., Springer, 2007.
5. B. Smith, J. March "Advanced Organic Chemistry" 6th Edn., Wiley-VCH, 2007.
6. E. J. Corey, X.-M. Cheng, "The Logic of Chemical Synthesis" Wiley-interscience, 1995.
7. T. Hudlicky, J. W. Reed, "The Way of Synthesis: Evolution of Design and Methods for Natural Products" Wiley-VCH, 2007.
8. P. Wyatt, S. Warren, "Organic Synthesis: Strategy and Control" Wiley, 2007.
9. Christmann, S, Brase Eds "Asymmetric Synthesis- The Essentials" 2nd Edn., Wiley-VCH, 2008.
10. K. C. Nicolaou, R. Hanko, W. Hartwig Eds. "Handbook of Combinatorial Chemistry", VCH-Wiley, Weinheim, 2002.

CHE742: Organic Chemistry Laboratory (84P Hours)

Coordinators: Dr. S. Peruncheralathan
peru@niser.ac.in

Course Details:

- Determination of strength of acid in lemon juice.
- Estimation of carbohydrates by anthrone method.
- Determination of isoelectric point of glycine.
- Paper and column chromatography of plant pigments: Extraction and separation of Chlorophyll A and Chlorophyll B.
- Separation of organic compounds from a mixture of compounds using the techniques of solvent extraction, preparative TLC and column chromatography and identification of the individual components by spectroscopic techniques (IR, NMR, UV-ViS), preparation of dry solvents.
- Synthesis of the following compounds using name reactions: a. Diels-alder reaction of anthracene and Maleic anhydride b. Synthesis of Cinnamic acid from Benzaldehyde (perkin reaction) c. Synthesis of Triphenyl Carbinol (Grignard Reaction) d. Synthesis of 2-hydroxy-5-methyl benzophenone (Fries rearrangement) e. Synthesis of Benzilic acid from Benzil (Benzil- Benzilic acid rearrangement) f. Synthesis of p-methoxycinnamic acid (Knoevenagel reaction).
- Synthesis of 2-phenylindole from acetophenone phenylhydrazone (Fischer-indole synthesis)
- Protection and deprotection technique: Synthesis of a ketal of cyclohexanone with ethylene glycol and regeneration of the ketone from the intermediate.
- Esterification of p-methoxycinnamic acid.
- Phenylacetylene from cinnamic acid (via dibromocinnamic acid and phenylpropiolic acid).
- Friedel Crafts Reaction and Wolff Kishner Reduction: 4-phenylbutyric acid from benzene (via – benzoylpropionic acid, and reduction of the carbonyl group employing hydrazine hydrate).
- 3-Hydroxycoumarin from glycine (via hippuric acid).
- Synthesis of Benzoimidazole,
- Synthesis of Caprolactam using Beckman rearrangement.
- Synthesis of Bisnaphthol.
- Synthesis of 3,4-dihydropyrimidin-2(1H)-ones using Biginelli reaction, a multiple-component chemical reaction.

Course Outcomes:

- Experience about synthesis of various biologically important molecules such as peptides, nuclease modification, quantification of amino acids and sugars.
- This course enables students to visualize the different techniques, principles, difficulties involved in synthesizing biomolecules

Reference:

1. An Introduction to Practical Biochemistry, D. T. Plumer, Tata Mcgraw Hill, 2000.
2. A Collection of Interesting General Chemistry Experiments, A. J. Elias, Universities Press, 2007.
3. Experimental Physical Chemistry: A Laboratory Textbook, A. M. Halpern and G. C. McBane, W. H. Freeman and Company, New York, 2006.
4. Vogels Textbook of Quantitative Chemical Analysis, G. H. Jeffery, J. Bassett, J. Mendham and R. C. Denny, 5th Edn., ELBS, 1991. Spectrometric Identification of Organic Compounds, R. M. Silverstein, G. C. Bassler and T. C. Morrill, 6th Edn., Wiley, 1998.

5. A Collection of Interesting general Chemistry Experiments, Anil J. Elias, Universities Press, 2007.
6. Laboratory Manual of Organic Chemistry, B. B. Dey and M. V. Sitaraman, Allied Publishers, 1992.
7. Laboratory Manual of Organic Chemistry, R. K. Bansal, New Age International Publishers, 2006.

2nd YEAR, SEMESTER-III

CHE801: Chemistry of Heterocycles and Natural Products ((45L+15T Hours)

Coordinators: Prof. C. Gunanathan
gunanathan@niser.ac.in

Course Details:

- **Chemistry of Heterocycles**
  Introduction and application of Heterocycles; Nomenclature of aromatic and non-aromatic Heterocycles; Synthesis and reactivity of 5&6-membered aromatic Heterocycles with One or Two hetero atoms.

- **Chemistry of Natural Products**
  Introduction and application of Carbohydrates; Steroids, Terpenoids, Fatty Lipids, Prostaglandins and alkaloids; Total synthesis of selected natural products.

Course Outcomes:

- Understanding nomenclature, structure and reactivity of aromatic and non-aromatic heterocycles.
- Understanding the design and application of various organic reactions for the synthesis of natural products.
- Understanding the classification, structure and synthesis of biomolecules

Reference:

1. J. A. Joule, K. Mills, "Heterocyclic Chemistry" 5th Edn., Blackwell, 2010.
2. T. Eicher, S. Hauptmann, "The Chemistry of Heterocycles" 2nd Edn., Wiley-VCH, 2003.
3. R. J. Simmonds, "Chemistry of Biomolecules: An Introduction" RSC, 1992.
4. I. L. Finar, "Organic Chemistry" Vol. II, ELBS, 1990.
5. S. V. Bhat, B.A. Nagasampagi, M. Sivakumar, "Chemistry of Natural Products" Springer, 2005.
6. E. J. Corey, X.-M. Cheng, "The Logic of Chemical Synthesis" Wiley-Interscience, 1995.
7. T. Hudlicky, J. W. Reed, "The Way of Synthesis: Evolution of Design and Methods for Natural Products" Wiley–VCH, 2007.

CHE802: Organometallic Chemistry (45L+15T Hours)

Coordinators: Prof. Sharanappa Nembenna
snembenna@niser.ac.in

Course Details:

- **General Properties of Organometallic Complexes**
  Werner Complexes; Trans Effect; Soft vs Hard Ligands; Crystal Field Theory; Back Bonding; Electroneutrality; Types of Ligands; 18 Electron Rule and Limitations; Electron Counting in Reactions; Oxidation State, Coordination Number and Geometry; Effects of Complexation; Difference between Metals; Outer Sphere Coordination. [6]

- **Complexes with σ-Bonded Ligands**
  Transition Metal Alkyls and Aryls; Related s-Bonded Ligands; Metal Hydride Complexes; s-Complexes and Bond Strength; Metal Complexes of CO, RNC, CS, NO, Phosphine and Related Ligands. [6]

- **Complexes with π-Bound Ligands**
  Alkene and Alkyl Complexes; Allyl Complexes; Diene Complexes; Cyclopentadienyl Complexes; Arenes and Other Alicyclic Ligands; Metalacycles; Polyene and Polyenyl Complexes. [6]

- **Ligand Substitution, Oxidative Addition and Reductive Elimination**
  Dissociative Substitution; Associative Mechanism; Redox Effect; Rearrangement in Substitution; Photochemical Substitution; Concerted Addition; SN2 Reaction; Radical Mechanism; Ionic Mechanism; Reductive Elimination; s-Bond Metathesis; Oxidative Coupling and Reductive Cleavage. [8]

- **Metal-Ligand Multiple Bonds**
  Carbenes; Carbynes; Bridging Carbenes and Carbynes; N heterocyclic Carbenes; Multiple Bonds to Heteroatoms. [5]

- **Application in Homogeneous Catalysis**
  Alkene Isomerization; Alkene Hydrogenation; Alkene Hydroformylation; Hydrocyanation; Alkene Hydrosilylation; Alkene Hydroboration; Coupling Reactions; Alkene Metathesis; Polymerization of Alkene. [6]

- **Application to Organic Synthesis**
  C-H Activation; Metal Alkyls, Aryls and Hydrides; Reduction and Oxidation; Protection and Deprotection; Reductive Elimination; Coupling Reaction; Insertion Reaction; Nucleophilic Attack on a Ligand. [5]

Course Outcomes:

- Understanding the reaction of coordinating metals with hydrocarbons.
- Useful to design the catalyst for C-H activation/functionalization.
- Applicable in the synthesis of target molecules in economically

Reference:

1. The Organometallic Chemistry of the Transition Metals, Robert H. Crabtree, Wiley, New York, Fourth Edition, 2005.
2. Organometallic Chemistry and Catalysis, Didier Astruc, Springer, New York, 2007. 3. Organometallic Chemistry, Gary O. Spessard and Gary L. Miessler, Oxford, Third Edition, 2015.
3. Basic Organometallic Chemistry: Concepts, Syntheses and Applications, B. D. Gupta and A. J. Elias, 2013.

CHE841: Physical Chemistry Laboratory (84P Hours)

Coordinators: Prof. Himansu S. Biswal
himansu@niser.ac.in

Course Details:

- Principles of bioinorganic Chemistry (Justification of why a certain protein/enzyme contains a particular metal ion). [3]
- Absorption, excitation and emission spectra of naphthalene, anthracene and indole to demonstrate the difference between absorption, excitation and emission.
- Fluorescence quenching of N-methylacridinium iodide (N-MEAI) with guanosine 5' monophosphate, disodium salt trihydrate (GMP), 1-pyrenesulfonic acid, sodium salt (PSA) with β-cyclodextrin (β-CD) and acetylnaphthalene (2-AN) with iodide ions to demonstrate static versus dynamic quenching.
- Study of the excited state properties of 2-naphthol: (a) excited state acidity constant; (b) deprotonation and protonation rate constants in the excited state.
- Variable temperature NMR experiment to study restricted bond rotation.
- Hammett correlations of amide proton chemical shifts.
- Keto–enol tautomerization of acetylacetone in mixed solvents by NMR spectroscopy.
- Kinetics study of a biotin analogue by using FT-IR spectroscopy.
- Investigating hydrogen bonding in Phenol and N-methylacetamide using FT-IR spectroscopy.
- Variable temperature UV-Vis. experiment to study the thermodynamics of DNA duplex formation.
- Determination of Isoelectric Point of proteins and nanomolecules with SDS-PAGE.
- Adsorption of methylene blue on activated carbon to investigate Langmuir and Freundlich isotherms.
- Adsorption of oxy-anions on iron oxide-titanium dioxide adsorbent.
- Optical properties of CdSe quantum dots.
- Introduction and hands on experience with solid-state and dye lasers.
- Laser induced fluorescence (LIF) spectra of anthracene and indole in supersonic jet condition: A comparative study with their solution phase fluorescence spectra (experiment -1).
- Illustration of Nernst equation by redox titration of Ferricyanide to Ferrocyanide with Ascorbic acid.

Course Outcomes:

- This is a lab course that introduces several spectroscopic methods to the students.
- Students can learn to use UV-Vis and fluorescence spectroscopy to determine pKa.
- To learn IR spectroscopy to monitor the progress of the reaction.
- To introduce the students NMR spectroscopy to study keto-enol tautomerism and kinetics.
- Introduces different electrochemical methods that are used in chemistry research

Reference:

1. Experiments in physical chemistry, 8th ed. / Carl W. Garland, Joseph W. Nibler, David P. Shoemaker, McGraw-Hill, 2009.
2. A Collection of Interesting General Chemistry Experiments, A. J. Elias, Universities Press, 2007.
3. Experimental Physical Chemistry: A Laboratory Text, 3rd ed. Arthur Halpern, George McBane, Publisher: W. H. Freeman; 2006. *** Integrated M. Sc-Ph. D at SCS, NISER (Page 21)
4. T. Engel and P. Reid, Physical Chemistry, Pearson, 2013.
5. P. W. Atkins and R. S. Friedmann, Molecular Quantum Mechanics, Oxford, 2008. 6. D. A. McQuarrie and J. D. Simon, Physical Chemistry – A Molecular Approach, Viva Books, New Delhi, 1998.

2nd YEAR, SEMESTER-IV

CHE803: Applied Spectroscopy (45L+15T Hours)

Coordinators: Dr. Bishnu P. Biswal
bp.biswal@niser.ac.in

Course Details:

- **Ultraviolet Spectroscopy**
  Electronic Transition; Definitions of related terms and designation of UV- absorption band; Studies of conjugated and extended conjugated systems; Woodward Fiesher rules; Analytical use of UV-spectroscopy.

- **Infrared and Raman Spectroscopy**
  Molecular Vibrations, Instrumentation of IR and Raman spectroscopic techniques; Interpretation of Infrared and Raman spectra, Identification of functional groups, Hydrogen bonding, Complexity of IR spectra, Utility of IR spectroscopy in structural elucidation. Raman spectroscopy in material science; SERS.

- **Fluorescence Spectroscopy**
  Phenomena of fluorescence; Photochemical laws; General characteristics; Quantum yield and its measurements; Radiationless transitions; Spin states and their interconversion; Kasha's rule and solvent effect; Spin orbit coupling; Energy transfer processes; Donor acceptor complexes, Excimers and Exiplexes. Fluorescence quenching (static and dynamic); Stern Volmer analysis; Timescale of molecular processes in solution. Steady state and time resolved fluorescence. Fluorescence anisotropy; Biochemical fluorophores; New fluorescence technologies: Multiphoton Excitation, Fluorescence correlation Spectroscopy, Single molecule detection.

- **Photoelectron Spectroscopy**
  Experimental methods, Ionisation processes and Koopmans theorem; Photoelectron spectra and their interpretation and applications.

- **Mass Spectrometry**
  Basic concepts; Instrumentation, Fragmentation and rearrangements (including McLafferty rearrangement) of different classes of organic molecules; Isotope effects.

Course Outcomes:

- Understanding the basics of absorption and fluorescence spectroscopy.
- Theoretical prediction of absorption maximum of some organic molecules.
- Identifying and distinguishing various type of electronic transition using solvent perturbation techniques.
- Understanding the concept of micro polarity and the importance of this parameter in spectroscopy.
- Understanding some important photo-processes such as electron transfer and energy transfer and their applications in energy related applications.
- Applications of fluorescence spectroscopy in detecting various analytes (Sensingapplications)

Reference:

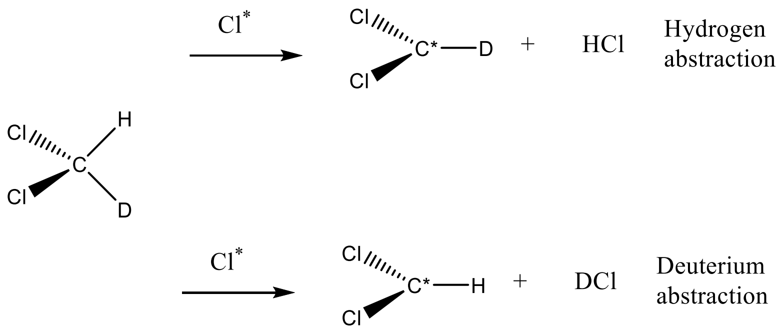
1. Modern Spectroscopy J. M. Hollas. Wiley, 2004.
2. Physical Methods in Chemistry, R. S. Drago, 2nd Edn., Saunders, 1992.
3. Essentials of Photochemistry, A. Gilbert and J. Baggot, Blackwell Scientific Publications, 1992.
4. Fundamentals of Photochemistry, K. K. Rohatgi Mukherjee, Wiley Eastern Ltd., 1978.
5. Molecular Fluorescence, Bernard Valeur, Wiley-VCH, 2002. *** Integrated M. Sc-Ph. D at SCS, NISER (Page 15)
6. Principles of Molecular Photochemistry: An Introduction, P. Walsh, N. J. Turro, V. Ramamurthy, J. C. Scaiano, University Science Books, 2008.
7. Principles of Fluorescence Spectroscopy. Joseph R. Lakowicz, 3rd Edn., Springer, 2006.
8. Interpretation of Mass Spectra, F. W. McLafferty, 1980.
9. Spectrometric Identification of Organic Compounds, R. M. Silverstein, G. C. Bassler and T. C. Morrill, John Wiley, New York.

CHE842: Computational Chemistry Lab (84P Hours)

Coordinators: Prof. U. Lourderaj
u.lourderaj@niser.ac.in

Course Details:

- Calculation of kinetic Isotope effects in chemical reactions using DFT methods. Example:



- Simulated vibrational, rovibrational and rotational Raman Spectra for diatomic molecules using spreadsheet. Example: HCl, N2
- Simulation of electronic spectra of simple molecules using CIS and TDDFT methods. Example: butadiene, hexatriene, and octatetraene
- Calculation of the first few eigenfunctions and eigenvalues of 1 dimensional harmonic and Morse oscillators using numerical methods such as the Numerov method. The Numerov method can be done using a spreadsheet or computer code.
- Calculation of the potential energy function for umbrella motion in ammonia using HF or DFT methods and fitting the energy data to an analytical form.
- Calculation of the first few eigenfunctions and eigenvalues for the double well potential developed in Lab 5 using Numerov method and hence the computation of tunnelling splitting in ammonia.
- Study of the relationship between HOMO-LUMO energy gaps, energy barriers and rate constants in Diels-Alder reactions using DFT methods.
- Study of the vibrational spectra protonated water cluster (dimer, trimer etc) and compare them with the experimental results such as Johnson's work. (Science, 299, 1375(2003).
- Activation energy, forward and backward rate constant and equilibrium constant for isomerization reactions to introduce Arrhenius equation and Eyring equation.

- Study of thermodynamic properties of Lennard-Jones fluids from molecular dynamics simulations.

- Application of Monte-Carlo simulations - Estimation of the value of π

Course Outcomes:

- Understanding the concepts of energy minimization, frequency calculations and transition state optimization
- Practical experience in applications of quantum chemical calculations
- Understanding of molecular dynamics and Monte-Carlo simulations using simple examples

Reference:

1. T. Engel and P. Reid, Physical Chemistry, Pearson, 2013.
2. N. Levine, Quantum Chemistry, Prentice-Hall of India, 2006.
3. P. W. Atkins and R. S. Friedmann, Molecular Quantum Mechanics, Oxford, 2008.
4. D. A. McQuarrie and J. D. Simon, Physical Chemistry – A Molecular Approach, Viva Books, New Delhi, 1998.

ELECTIVE COURSES

CHE901: Photochemistry (45L+15T Hours)

Coordinators: Dr. S. Peruncheralathan
peru@niser.ac.in

Course Details:

- **Introduction**
  Importance of photochemistry; Electromagnetic Radiation; Color perception and the Colour Circle; Beer–Lambert Law; Electronic Configurations: Multiplicity, S0, S1, T1 etc.; Electronic Transitions and Solvent Effects: π to π*, n to π* etc. Molecular Orbitals (FMO Approach).

- **Unimolecular Photophysical Processes**
  Jablonski Diagram; Frank–Condon principle; Fluorescence; Intersystem Crossing; Phosphorescence; Delayed Fluorescence; Quantum Yield.

- **Bimolecular Photophysical Processes**
  Thermodynamics and Kinetics of Excited State Bimolecular Interactions; Excimer and Exciplex; Photosensitization and Quenching; Heavy atom Effect; Photoinduced Electron and Charge Transfer; Resonance Energy Transfer: Coulombic and Exchange Mechanisms.

- **Fluorescence Spectroscopy**
  Characteristics of Excitation and Emission Spectra; Basic Theories involving Various Fluorescence Spectral parameters; Fluorescence anisotropy; Introduction to Fluorescence probing Techniques and Applications; Fluorescent Molecular Sensors of Ions and Molecules.

- **Photochemistry of Organic Compounds**
  Photochemistry of alkenes; Pericyclic Reactions; Photo-oxidation and photo-reduction; Photochemistry of Carbonyl Compounds.

- **Photochemistry of Organic Compounds**
  Chemistry of Vision; Photochemistry in nature; Photochemistry in atmosphere; Supramolecular photochemistry; Solar Cell; Fuel cell.

Course Outcomes:

- Understanding the photoinduced reactions in chemical and biological systems.
- Understanding the photo-physical processes.
- Basic principles and application of fluorescence spectroscopy.
- Use the knowledge of photochemistry in materials applications

Reference:

1. Fundamentals of Photochemistry, K. K. Rohatgi Mukherjee, Wiley Eastern Ltd., 1978.
2. Modern Molecular Photochemistry, N. J. Turro, University Science Books, 1991.
3. Molecular Fluorescence, B. Valeur, Wiley-VCH,2002.
4. Principles of Molecular photochemistry: an introduction, P. Walsh, N. J. Turro, V. Ramamurthy, J. C. Scaiano, University Science Books, 2008.
5. Organic photochemistry, J. M. Coxon and B. Halton, Cambridge University press, 1974.
6. Molecular Reactions and Photochemistry, C. H. Depuy and O. L. Chapman, Prentice Hall of India.
7. Photochemistry and Pericyclic Reactions, J. Singh and J. Singh, New Age International Publishers, 2003.
8. Pericyclic Reactions, I. Fleming, Oxford Science Publications 1998.

CHE902: Pharmaceutical Chemistry (45L+15T Hours)

Coordinators: Dr. S. Peruncheralathan
peru@niser.ac.in

Course Details:

- **Drug discovery and development**
  The why and wherefore of drugs; Stereochemistry and solubility factors; Principles of drug design (molecular and biochemical); 'Lead' modification approach, SAR/QSAR; Computer-aided drug design; Natural products drug discovery.

- **Basic principles of medicinal chemistry**
  Drug action at enzymes; Drug action at receptors; Physico-chemical aspects of drug molecules; Selected examples of drugs and natural products.

- **Pharmacodynamics and pharmacokinetics**
  Drug distribution and survival; Concept of prodrug; Pharmacokinetic models; Drug metabolism.

Course Outcomes:

- To learn pharmacokinetics and pharmacology.
- To understand pharma cores and their interactions in molecular targets.
- To interpret AMDE principle of drugs (absorption, distribution, metabolism, and excretion).
- To understand drug discovery processes.

Reference:

1. Essentials of Pharmaceutical Chemistry, D. Cairns, Pharmaceutical press, 2nd Edition 2003.
2. Fundamentals of Medicinal Chemistry, G. Thomas, Wiley-Blackwell, 1st Edition, 2003.

CHE903: Classics in Molecules (45L+15T Hours)

Coordinators: Dr. S. Peruncheralathan
peru@niser.ac.in

Course Details:

- Introduction, Understanding structural diagrams of organic molecules, Protein and Three-dimensional protein Structure, Nucleic acids, Synthesis, Biosynthesis.
- Urea & acetic acid, glucose, aspirin, Camphor, Terpineol, Tropinone, Haemin, Quinine, Morphine, Steroids & the pill, Strychnine, penicillin, Longifolene, prostaglandins & Leukotrienes, Vitamin B12, Erythronolide B & Erythromycin a, Monensin, Avermectin, Amphotericin B, Ginkgolide B,
- Cyclosporin, FK506 & Rapamycin, Calicheamicin γ1, Palytoxin, Taxol, Mevacor, Zaragozic acids & Cp Molecules, Brevetoxin B, Ecteinascidin 743, Epothilones, Resiniferatoxin, Vancomycin, Thiostrepton.
- Modern Drug Discovery and Developments, Designed Small Drug Molecules for Mental illness, Viral infections, gastrointestinal Disorders, Heart diseases and Sexual Dysfunction.
- DNA Technologies, Vaccines, antibodies, Diabetes, anemia, Rheumatoid arthritis, Breast Cancer, Biologics.

Course Outcomes:

- To learn discovery of organic molecules and their impact on the world such as Urea, Glucose, & Penicillin.
- To understand the basic organic chemistry for learning chemical biology.
- To learn the small organic molecules that interaction with molecular targets.
- To find the nature of drugs and their function in biological changes.

Reference:

1. K. C. Nicolaou and Tamsyn Montagnon, “Molecules that Changed the World”, Wiley-VCH, 2008.
2. E. J. Corey, László Kürti and Barbara Czak´o, “Molecules and Medicine”, Wiley-VCH, 2008.
3. J. Block and J. M. Beale “Wilson and Gisvold’s Textbook of Organic Medicinal and Pharmaceutical Chemistry”, 11th Edn., Lippincott Williams & Wilkins, 2003.

CHE904: Molecular Modeling (45L+15T Hours)

Coordinators: Prof. U. Lourderaj
u.lourderaj@niser.ac.in

Course Details:

- **Introduction**
  What is molecular modeling? Computable quantities.

- **Concept of Potential Energy Surface**
  Stationary points, Born–Oppenheimer approximation, Geometry optimization, Normal modes of vibration

- **Molecular Mechanics**
  Basic principles, properties that can be calculated, Strengths and weaknesses.

- **Quantum Mechanics**
  Unimolecular and Bimolecular reactions, Reaction path and transition states, Classical trajectories, Direct dynamics, Quantum dynamics.

- **Simulations of Molecular Ensembles**
  Properties as ensemble and time averages, Molecular dynamics simulations, Monte Carlo simulations.

- **Modeling Lab**
  Hands-on experience for using different simulations methods and algorithms pertaining to the course.

Course Outcomes:

- Construction of potential energy surfaces and force-fields for molecules
- Perform HF, DFT, and semi-empirical calculations on molecules
- Perform chemical dynamics simulations for simple reactions
- Apply molecular dynamics and Monte-Carlo simulations on large sized molecules

Reference:

1. N. Levine, Quantum Chemistry, Prentice-Hall of India, 2006.
2. P. W. Atkins, Molecular Quantum Mechanics, Oxford, 2008.
3. P. Allen and D. J. Tildesley, Computer Simulation of Liquids, Oxford, 1987.
4. R. Leach, Molecular Modelling, Prentice Hall, 2001.
5. F. Jensen, Introduction to Computational Chemistry, John Wiley & Sons, 2007.

CHE905: Solid State Chemistry (45L+15T Hours)

Coordinators: Prof. J. N. Behera
jnbehera@niser.ac.in

Course Details:

- **Crystal Chemistry**
A brief introduction to crystallography, Lattices, unit cells, symmetry, point groups, space groups. packing: CCp, HCp, voids, radius ratio rules. Bonding in crystals: ionic, covalent, metallic, van der Waals, hydrogen bonds. Description of crystal structures: metallic & non metallic structures, AB, AB2, AB3 (ReO3), spinels, pyrochlores, perovskites, K2NiF4 etc. Pauling's rules for ionic crystal structures and the concept of bond valence. Methods of crystallography: powder, single crystals, X-ray, neutron and electron diffraction.

- **Defects in Solids**
Origin of defects in crystals; perfect and imperfect crystals; thermodynamics of defect formation; types of defects: point defects, line defects, plane defects; Schottky and Frenkel defects; thermodynamics of Schottky and Frenkel defect formation; crystal classifications; Madelung constant and lattice energy.

- **Electronic Structure of Solids**
Atoms to molecules to crystals; Orbitals to bonds to bands; Electronic structure of crystalline solids, Elementary band theory: Metals, Insulators and Semi-conductors., Solid state ionics; Intrinsic and Extrinsic semiconductors. Transport property measurement techniques: Electrical resistivity, Thermopower, Hall effect Magnetism of d vs. f block metal compounds

- **Critical Phenomena**
Phase transitions (Order-disorder, Martensite-austenite, Spinodal decompositions); Liquid crystals; Structure–property relations (magnetic, electrical, superconductivity, optical and thermal); Powder synthesis by conventional and modern chemical methods; Reactivity of solids; Decomposition mechanisms; Powder processing (sintering and diffusion processes), Tailoring of solids, Special methods for single crystal growth and thin film depositions.

- **Synthesis of Solids**
Chemistry behind synthesis; Intercalations; Synthesis/preparation of single crystals; Hydrothermal methods. Framework Solids; Zeolites, Aluminophosphates and related structures; Metal-organic framework compounds – their structures and properties.

- **Superconductivity**
General aspects of superconductivity; Effects of magnetic field; BCS Theory; Oxide Superconductors.

Course Outcomes:

- Describe the principles concerning solid state structures
- Describe specific crystal structures by applying basic crystallographic concepts
- Describe the experimental use of the diffraction phenomenon
- Use powder diffraction data for characterising cubic substances
- Analyse thermograms and phase diagrams in known systems

Reference:

1. Solid State Chemistry and Its Applications, A. R. West, John Wiley, 1987.
2. Solid State Chemistry, L. Smart and E. Moore, Chapman and Hall, 1992.
3. Principles of the Solid State, H. V. Keer, Wiley Eastern Ltd., 1994.
4. New Directions in Solid State Chemistry, C. N. R. Rao and J. Gopalakrishnan, Cambridge University Press, 2008.
5. The Electronic Structure and Chemistry of Solids, P. A. Cox, Oxford University Press, 2005.
6. Ionic crystal, Lattice defect and Non-stoichiometry, N. N. Greenwood, Chemical Pub. Co., New York, 1970.
7. An Introduction to Crystal Chemistry, R. C. Evans, Cambridge University Press, 1964.

CHE906: Crystallography (45L+15T Hours)

Coordinators: Prof. J. N. Behera
jnbehera@niser.ac.in

Course Details:

- Origin of X-rays, Filters, Monochromators, Sealed tube, Rotating anode synchrotron radiation, Safety considerations.

- Crystals and their properties- Concepts of symmetry, Direct and reciprocal lattice, Planes, Indices, Unit cell, Bragg's law in direct and reciprocal lattices, Primitive and non-primitive lattices, Point and space groups, Equivalent positions, Systematic absences and space group determination, Occupancy factors.

- Theory of structure factors, Argand diagram and its use, Lorentz and polarization corrections, Absorption corrections, Absolute scale of intensities; Unit cell determination, Data collection parameters, Data reduction, Phase problem and structure solution by Patterson and direct methods.

- Structure refinement techniques, Presentation and interpretation of structural data, Examination of CIF file and critical evaluation of a structure, Errors and pitfalls, Twinning and disorder, Renninger effect, Extinctions, Anomalous scattering and its use.

Course Outcomes:

- Define concepts such as lattice, point and space groups
- Be familiar with Bragg's Law and explain its relation to crystal structure
- Identify and describe different diffraction methods
- Interpret and assign X-ray and electron diffraction patterns
- Use crystallographic data for a validated phase analysis

Reference:

1. X-Ray Structure Determination: A Practical Guide, G. H. Stout and L. H. Jensen, Springer, 1992.
2. Fundamentals of Crystallography, C. Giacavazzo, Oxford University Press.
3. X-Ray Analysis and the Structure of Organic Molecules, Jack. D. Dunitz, Wiley, 1996.
4. Crystal Structure Determination, Werner Massa, Springer.
5. Structural Inorganic Chemistry, A. F. Wells, Clarendon Press, 1986.

CHE907: Principles of Drug Action (45L+15T Hours)

Coordinators: Dr. S. Peruncheralathan
peru@niser.ac.in

Course Details:

- **Pharmacodynamic Phase in Drug Action**
  Introduction to pharmacodynamics, Biochemical basis of drug action, Drug absorption, distribution and bioavailability, Passive diffusion, Active transport mechanisms, Excretion and reabsorption of drugs.

- **Pharmacokinetic Phase in Drug Action**
  General classification of pharmacokinetic properties, Pharmacokinetic models, Intravascular administration, Extravascular administration, Estimation of pharmacokinetic parameters, The use of pharmacokinetics in drug design.

- **Novel Therapeutic agents: Synaptic Pharmacology**
  Cholinergic and adrenergic systems, CnS agents: Antipsychotics, Antidepressants, CVS Agents: Antihypertensives, Antineoplastic agents, Analgesic and anti-inflammatory agents, Drug toxicity.

- **Concepts in Drug Metabolism**
  Basic principles and factors affecting drug metabolism, Secondary pharmacological implications of metabolism, Phase i metabolic reactions, Phase ii metabolic reactions, Drug metabolism and drug design, Prodrugs, Metabolic pathways for common drugs.

- **Stability of Drugs and Medicines**
  Oxidation and stability of free-radicals, Prevention of oxidative deterioration, Autoxidation of fats and oils, Examples of drugs susceptible to aging and hydrolysis, Other mechanisms of degradation.

- **Drug Development**
  Clinical trials (phase-i to phase-iv), Formulation development, Quality control aspects (methods of assay).

Course Outcomes:

- To learn pharmacokinetics and pharmacology
- To understand absorption, distribution, metabolism, and excretion of drugs
- To learn various stages of drug discovery process such as clinical trails
- To find the modern drug discovery and development processes including the identification of molecular targets, High-throughput screening (HTS)

Reference:

1. Thomas G. (2003) Fundamentals of Medicinal Chemistry, Wiley.
2. Cairns D. (2008) Essentials of Pharmaceutical Chemistry (3rd Edn.), Pharmaceutical Press.
3. Block J. and Beale J. M. (2003) Wilson and Gisvold's Textbook of Organic Medicinal and Pharmaceutical Chemistry (11th Edn.), Lippincott Williams & Wilkins.
4. Rang H. P., Dale M. M. et al. (2007) Rang & Dale's pharmacology (6th Edn.), Churchill Livingstone.
5. Hardman J. G., Limbird L. E. et al. (2001) Goodman & Gilman's. The pharmacological Basis of Therapeutics, Mcgraw-Hill Professional.

CHE908: Advanced Bio-inorganic Chemistry (45L+15T Hours)

Coordinators: Prof. Sanjib Kar
sanjib@niser.ac.in

Course Details:

- Principles of bioinorganic Chemistry (Justification of why a certain protein/enzyme contains a particular metal ion).

- **Heme Proteins**
  Types, function and mechanisms, Myoglobin, Hemoglobin, Cytochrome C, Cytochrome-P450, Peroxidases (Horseradish peroxidase, Chloroperoxidase), Catalase, Cytochrome C Oxidase, Synthetic porphyrins of biological relevance.

- **Non-Heme Proteins**
  Types, function and mechanisms, Mononuclear Systems (Catechol-1,2-Dioxygenases, Transferrin, Ferritin, Superoxide Dismutase, Isopenicillin N Synthase) Dinuclear Systems (Hemerythrin, Ribonucleotide Reductase, Methane Monooxygenase, Purple acid phosphatases).

- **Heme Proteins**
  Types, function and mechanisms, Myoglobin, Hemoglobin, Cytochrome C, Cytochrome-P450, Peroxidases (Horseradish peroxidase, Chloroperoxidase), Catalase, Cytochrome C Oxidase, Synthetic porphyrins of biological relevance.

- **Copper Proteins (Type i, ii, and iii)**
  Types, function and mechanisms, Blue Copper proteins; Hemocyanin, Tyrosinase, Catechol Oxidase; Superoxide Dismutase; ascorbate Oxidase, Laccase; galactose oxidase

- **Molybdenum Enzymes**
  Types, function and mechanisms, Oxo-Transfer Enzymes, Xanthine Oxidase, Nitrogenase.

- **Manganese**
  Photosynthesis (Photosystem I and Photosystem II); function and mechanisms.

- **Zinc Enzymes**
  Function and mechanisms, Hydrolytic Enzymes (Carbonic anhydrase; Carboxypeptidase A; Alkaline phosphatase).

- **DNA/RNA**
  Types, function and mechanisms, DNA nicking enzymes; DNA polymerase; Ribozymes.

- **Environmental & Medicinal Aspects**
  Acid-rain; Green-house Effect etc. Radiopharmaceuticals; Photodynamic Therapy; Anti-Tumor Drugs (cis-platin, Carboplatins; Bleomycins); Ion-pumps.

Course Outcomes:

- Apply the basic principles in inorganic and general chemistry to interdisciplinary topics in the field of bio-inorganic chemistry.
- Describe the main roles of metal ions in biological processes and identify the chemical properties that are required to each particular function.
- Describe the role of metal ions in enzymes involved in acid-base reactions.
- Describe the role of metal ions that are involved in electron-transfer reactions in biological systems.
- Describe how oxygen is transported in different species and identify the metal centers involved in this task.
- Describe the different metal-activation sites in enzymes that are involved in the activation of oxygen.
- Identify the main toxicological mechanisms of metals and the biological defenses against the toxic effects.
- List some medical applications of inorganic compounds.
- Oral and written communication using the specific language of bioinorganic chemistry and common.

Reference:

1. Principles of Bioinorganic Chemistry; S. J. Lippard and J. M. Berg, Panima Publications, New Delhi, 1997.
2. Bioinorganic Chemistry; Inorganic Elements in the Chemistry of Life; W. Kaim, B. Schwederski Wiley, 1994.
3. Biological Inorganic Chemistry: Structure and Reactivity; Harry B. Gray, Edward I. Stiefel, Joan Selverstone Valentine, Ivano Bertini, University Science Book; 2006.
4. Specific Review Articles to be collected from the Internet.

CHE909: Nuclear Magnetic Resonance (45L+15T Hours)

Coordinators: Dr. Arindam Ghosh
aringh@niser.ac.in

Course Details:

- **Classical NMR Spectroscopy**
  Nuclear magnetism, Bloch equations, Chemical shift, Linewidth, Scalar coupling.

- **Theoretical description of NMR spectroscopy**
  Expectation value of magnetic moment, Density matrix, Pulses and rotation operator, Chemical shift and coupling Hamiltonians, Concept of coherence, One pulse experiment.

- **Product Operator Formalism**
  Operator spaces, Basis operators, Free precision, Pulses, Single and multiple quantum coherences, Application of pOF to study spin echo and standard polarization transfer protocols like in EpT.

- **Practical Aspects of NMR Spectroscopy**
  Tuning, Matching, Shimming, Temperature calibration, Spectrum referencing, Sampling theorem, Quadrature detection, Fourier transformation, Zero filling, apodization, Phasing, Signal to noise ratio, Spin decoupling, Pulse field gradients, Water suppression, One dimensional experiment.

- **Two-dimensional NMR Experiments**
  Two-dimensional spectroscopy, Coherence transfer, COSY, double quantum filtered COSY, TOCSY, NOESY, HSQC, HMQC, Sensitivity enhanced HSQC.

- **Higher-dimensional NMR Experiments**
  Need for higher dimensional experiments, HNCA, HN(CO)CA, introduction to the new trend of fast multidimensional experiments: GFT, spatially spatial encoding.

Course Outcomes:

- Theoretical understanding of the basic working principle of NMR spectroscopy.
- Building in-depth knowledge of the routinely performed experimental steps.
- Analysis of pulse sequence of few key one- and two-dimensional experiments to understand how certain spectra are generated.
- Understanding the theory behind common problems encountered during routine operation of an NMR spectrometer

Reference:

1. Protein NMR Spectroscopy, 2nd Edn., John Cavanagh, W. J. Fairbrother, A. G. Palmer.
2. M. Ranceand N. J. Skelton, Elsevier Academic Press, 2007.
3. Spin dynamics 2nd Edn., Malcolm H. Levitt, John Wiley and Sons Ltd., 2008.

CHE910: Advanced Functional Materials (45L+15T Hours)

Coordinators: Prof. Sudip Barman
sbarman@niser.ac.in

Course Details:

- **Introduction to Materials in Modern Technology**
  Materials as an enabling element of technological progress; Functions that materials perform; The properties - structure - processing connection.

- **Semiconductor Materials**
  Intrinsic semiconductors, Band Structure of Semi- conductors, Impurity Semiconductors, ii-v and ii-vi compounds, Hall effect, SC devices. Charge carrier dynamics in semiconductor nanomaterials.

- **Dielectric Materials**
  Dielectric constant and polarizability, Insulating materials, Ferroelectrics, piezoelectrics, Measurement of Dielectric properties, Applications.

- **Nanosized Magnetic Materials**
  Basic concepts of magnetism; Types of magnetic behavior, Magnetic domains, Soft and hard magnets, Classification of magnetic nanomaterials, Ferrofluids, Single-domain particles, Physical Properties of Magnetic nanostructures, Nano magnetism for biological applications.

- **Polymer Materials and Nano-composites**
  Classification of Polymers, Structure–Property Correlation, Molecular weights, Conduction in polymers, Natural composites, Incorporation of nanomaterials into polymer Media, Organic polymer nanocomposites, Metal and Ceramic composites, Clay nanocomposite Materials, Polymer–Clay nanocomposites, Polymer/graphite nanocomposites, Polymer Composites with Carbon nanotubes.

- **Amorphous and Crystalline Porous Materials**
  Crystalline vs. Amorphous Solids, Glass Formation, Structural models of amorphous materials, Properties of meta glasses, Evolution and Development of porous materials, Chemistry of microporous materials, Mesoporous materials, Semiconductor nanoparticles in Zeolites, Polymers and carbon materials in Zeolites.

Course Outcomes:

- Introduction to materials in modern technology
- Learn about semiconductor and dielectric materials
- Exploring the role of magnetic materials in inter-disciplinary sciences
- Use of polymer materials and nanocomposites in chemistry and day-today life

Reference:

1. Fundamentals of nanotechnology, Gabor L. Hornyak, John J. Moore, Harry F. Tibbals, Joydeep Dutta, CRC Press, Taylor & Francis Group, 2009.
2. Optical Properties and Spectroscopy of Nanomaterials, Jin Z. Zhang, World Scientific Publishing Co. Pte. Ltd, 2008.
3. Science of Engineering Materials and Carbon nanotubes, C. M. Srivastava, C. Srinivasan, New Age International Publishers.
4. Optimization of Polymer Nanocomposite Properties, Edited by Vikas Mittal, WILEY-VCH Verlag gmbH &Co. KGaA, Weinheim, 2009.
5. Polymer Nanocomposites Handbook; Rakesh K. Gupta, Elliot Kennel, Kwang-Jea Kim, CRC Press, Taylor & Francis Group, 2008.

CHE911: Supramolecular Chemistry (45L+15T Hours)

Coordinators: Dr. C. S. Purohit
purohit@niser.ac.in

Course Details:

- **Introduction**
  Understanding of Supramolecular Chemistry (Multidisciplinary nature, Complementarities in biology); Selectivity; Supramolecular interactions; Chelate and Macrocyclic Effects; Characterizing Supramolecular Systems; Structural, Kinetic and Thermodynamic.

- **Molecular Self-assembly**
  Non-Covalent Interactions: Electrostatic, Hydrogen Bonding, π−π Stacking, Dispersion and Induction Forces, Hydrophobic or Solvophobic Effects, π-Electron Donor–Acceptor Systems, Catenanes and Rotaxanes, Transition Metal Directed assemblies; Molecular Macrocycles and Boxes: Locked and Unlocked Molecular Boxes, Ladders and grids, Cages; Hydrogen Bond Directed assemblies: Rosettes and Ribbons, peptide nanotubes; Self-Replicating Molecular Systems.

- **Synthesis of Macrocycles**
  High Dilution Technique; Coordination Template Effects; Cation Binding and Demetallation; Porphyrins; Corrins; Crown Ethers; Cryptands; Spherands; Sepulchrates; Siderophores; Calixarenes. [

- **Molecular Sensors of Ions and Molecules**
  Anions, Cations and Neutral molecules receptor design principles: Recognition by electrostatic and hydrogen bonding, Lewis acidic Hosts interactions etc.; Introduction to fluorescence probing techniques and applications: Fluorescent molecular sensors of ions and Molecules, Logic gate etc.; Expanded porphyrins, Amide functionalized metallo compounds, Cyclophanes, Electrostatics and

- Hydrophobicity, Hydrogen bond receptors, Chiral recognition; Hydrophobic effect: Recognition in water; Solvent effect; Cyclodextrins; Calixarenes; Metallo receptor for nucleic acid and bases; Boronic acid receptors for Sugars.

Course Outcomes:

- Learn various noncovalent interactions
- Design the synthesis of novel macrocycles
- Understand the stabilization of anions, cations and neutral substrates
- To evaluate the binding and stability constants

Reference:

1. D. J. Cram and J. M. Cram, Container Molecules and their Guest, Monographs in Supramolecular Chemistry, Ed. J. F. Stoddart, The Royal Society of Chemistry, Cambridge, 1994.
2. J. M. Lehn, Supramolecular Chemistry: Concepts and Perspectives, VCH, Weinheim, 1995.
3. Comprehensive Supramolecular Chemistry, Edn. J. L. Atwood, J. E. D. Davies, D. D. Macnicol, F. Vogtle, Volumes 2 and 3, Elsevier Science, Oxford, 1996.
4. Supramolecular Chemistry of Anions, Edn. A. Bianchi, K. Bowman-James, E. Garcia- Espana, John Wiley and Sons, New York, 1997.
5. Supramolecular Chemistry, P. D. Beer, P. A. Gale and D. K. Smith, Oxford University Press, 1999.
6. A Practical Guide to Supramolecular Chemistry, Peter J. Cragg, John Wiley & Sons Ltd, England, 2005.

CHE912: Chemistry of Nanomaterials (45L+15T Hours)

Coordinators: Prof. Sudip Barman
sbarman@niser.ac.in

Course Details:

- **Introduction**
  Nano and nature, Fascination and Motivation of nanoparticle research, Bottom-up and Top-down approaches.

- **Zero and One-Dimensional Nanostructures**
  Introduction, aqueous and non- aqueous sol-gel chemistry, Surfactant-assisted synthesis, Solvent-controlled nanoparticles assembly: Introduction, Oriented attachment and Mesocrystals, Superlattices, Core-Shell nanoparticles: introduction, Types of systems, Characterization, properties. [10]

- **Carbon Nanomaterials**
  Fullerenes and their derivatives, Carbon nanotubes: Structure and properties, nanocrystalline diamond.

- **Self-assembled Monolayers**
  Introduction, Monolayers on gold, Growth process, Phase transitions, Patterning monolayers, Mixed monolayers structure, Electrochemistry and applications of self-assembled monolayers of thiols.

- **Nano and Micro-emulsion**
  Surface active agents, Micellization, Mechanism of emulsion, Characterization of Microemulsion.

- **Application of Nanomaterials**
  Solar energy conversion, Molecular and nano-electronics, Nanocatalyis, Biological applications and other applications.

Course Outcomes:

- Key concepts of Bottom-up and Top down approaches
- Understanding the mechanism of formation of 0-D, 1-D, 2-D, 3-D
- Nanostructured materials
- Understanding the structure-property relationship of carbon nanomaterials and self assembled monolayers
- Application of nanomaterials for energy applications and biological applications

Reference:

1. Nanoparticles: Synthesis, Stabilization, Passivation, and Functionalization, Edited by R. Nagarajan, T. Alan Hatton, ACS Symposium Series 996.
2. Metal Oxide Nanoparticles in Organic Solvents, Markus Niederberger and Nicola Pinna, Springer-Verlag London Limited, 2009.
3. Fundamental of Nanotechnology, Gabor L. Hornyak, John J. Moore, Harry F. Tibbals, Joydeep Dutta, CRC Press, Taylor & Francis Group, 2009.
4. Carbon Nanomaterials, Advanced Materials Series, Edited by Yury Gogotsi, Taylor and Francis Group, LLC, 2006.

5. Carbon Nanotubes and Related Structures, Edited by Dirk M. Guldi and Nazario Martin, WILEY– VCH Verlag GmbH & Co. KGaA, Weinheim, 2010.
6. Nano: The Essential, Understanding Nanoscience and Nanotechnology, T. Pradeep, Tata Mcgraw–Hill publishing Company Limited.
7. Applied Surfactants, Thrwat F. Tadros, WiLEY-VCH Verlag gmbH & Co. KGaA, Weinheim, 2006.

CHE913: Advanced Bio-organic Chemistry (45L+15T Hours)

Coordinators: Dr. N. K. Sharma
nagendra@niser.ac.in

Course Details:

- **Enzymology**
  Mechanistic studies of enzymatic reactions. Studies of enzyme kinetics for substrate/inhibitors (reversible/irreversible) and their future aspects in drug design. The role of cofactors and hormones in enzymatic reactions. Enzymes as Catalysts in organic chemistry reaction (group Transfer Reactions, Reduction and Oxidation; Monooxygenation; Dioxygenation Substitutions, Addition/Elimination; Carboxylations; Decarboxylation; isomerizations; aldol and Claisen Reactions; and Retro-reactions; Formylations, Hydroxy methylations, and Methylations; rearrangements.

- **Application of Enzyme Kinetics**
  Substrate Kinetics; Kinetics of Enzyme inhibition; Substrate inhibition; Non-productive Binding; Competing Substrates; Multi-substrate Systems; Allosterism and Cooperativity.

- **Biosynthesis of Secondary Metabolites**
  Polyketide Biosynthesis; Saccharide Biosynthesis; Shikimate pathway (pDF); Shikimate pathway Flavonoids; alkaloid Biosynthesis; Alkaloid Biosynthesis: Tyrosine Derivatives; Terpene Biosynthesis with example-Taxol, Vancomycin, Penicillin and other recent discovered natural products; Design and synthesis of modified secondary metabolites analogues; Isotope labeling (radioactive/non-radioactive) and their application in biosynthetic pathways.

- **Non-natural Bio-active Molecules**
  Synthesis and importance of these amino acids (β, γ & δ), non-ribosomal peptides and nucleotides (PNA, LNA, TNA & other stable analogues).

- **Introduction of Vital Bio-macromolecule Secondary Structures**
  g-Quadruplex, i-motif, RNAi (mi-RNA & si-RNA) & Collagen and their application in therapeutics.

Course Outcomes:

- Introduction of Bio macromolecules, and Enzymology
- Synthesis and application of DNA, RNA and related analogues
- Attract for biosynthesis of natural products
- Impress the role bio macromolecules in therapy

Reference:

1. Organic Chemistry of Enzyme-Catalyzed Reactions, Revised Edition by Richard Silverman, Academic Press, 2002.
2. Structure and Mechanism in Protein Science: A Guide to Enzyme Catalysis and Protein Folding Byalan Fersht, Publisher: W. H. Freeman; 1998.
3. Evaluation of Enzyme Inhibitors in Drug Discovery: A Guide for Medicinal Chemists and Pharmacologists (Methods of Biochemical Analysis); by Robert A. Copeland, Publisher: Wiley- interscience; 2005.

4. Dewick, Paul M. Medicinal Natural Products: A Biosynthetic Approach. 2nd Edn.. New York, NY: John Wiley & Sons, 2001.
5. Structural Diversity of g-Quadruplex Scaffolds; Stephen Neidle and Shankar Balasubramanian, CRC Press, 2006.
6. Gene Silencing by RNA Interference: Technology and Application, by Muhammad Sohail (Editor), CRC Press, 2004.
7. Modified Nucleosides: in Biochemistry, Biotechnology and Medicine (ed P. Herdewijn), Wiley-VCH Verlag GmbH &Co. KGaA, Weinheim, Germany.
8. Natural products: The Secondary Metabolites, James R. Hanson, RSC, 2003.

CHE914: Polymer Chemistry (45L+15T Hours)

Coordinators: Prof. V. Krishnan
krishv@niser.ac.in

Course Details:

- Classification of polymers, Nomenclature of polymers, Synthesis of polymers using different methods, viz Chain polymerization, Step polymerization, Ring-opening polymerization etc. Polymerization techniques, viz bulk polymerization, Solution polymerization, Suspension polymerization, Emulsion polymerization etc.

- Polymer characterization, molecular weight-number average, weight average; significance of molecular weight; Methods of characterizing molecular masses, GPC, Viscosity, Mass analysis, End-group analysis, Thermal properties - melting point, Glass transition temperature (Tg), Factors influencing Tg, relation between Tg and molecular weight, Crystallinity in polymers - degree of crystallinity in polymers, Structural regularity and crystallinity.

- Kinetics of polymerization, Free-radical, Cationic and Anionic polymerization and polycondensation. [5]

- Copolymerization, Free-radical and ionic copolymerization and Copolycondensation.

- Stereochemistry of polymerization, Types of stereoisomerism in polymers, Properties of stereoregular polymers, Different methods for the synthesis of stereoregular polymers; Less traditional approaches: aTRp, RaFT, ROMp, Surface functionalization of polymers.

- Biodegradable polymers: Synthesis and challenges.

Course Outcomes:

- Different types of polymers
- Concepts of polymers
- Applications of polymers
- Challenges involved in making bio-degradable polymers

Reference:

1. Odian, G. Principles of Polymerization. 4th Edn. Hoboken, NJ: Wiley-interscience, 2004.
2. Allcock, H. R., Lampe, F. W. in Contemporary Polymer Chemistry; Prentice-Hall: Englewood Cliffs, NJ, 1990.
3. Billmeyer Jr. F. W. Textbook of Polymer Science Wiley-interscience

CHE915: Molecular Reaction Dynamics (45L+15T Hours)

Coordinators: Prof. U. Lourderaj
u.lourderaj@niser.ac.in

Course Details:

- **Introduction**
  The rate constant - History and current view. What are molecular reaction dynamics?

- **Theoretical methods i**
  Transition State Theory (TST), RRKM Theory

- **Theoretical methods ii**
  Rate and cross-section, Classical scattering theory, Quantum scattering theory (reactive and non-reactive), Connection to TST and RRKM.

- **Experimental methods**
  Newton's diagrams, Molecular Beams, State-resolved spectroscopic techniques, Imaging techniques.

- **Applications**
  Photoselective chemistry - photodissociation and photoisomerization dynamics, Dynamics in real time (ps, fs and attosecond regimes), Molecular energy transfer, Control of chemical reactions, Condensed phase dynamics, Dynamics of gas-surface reactions.

Course Outcomes:

- Apply the transition state theory and RRKM theory to compute rate constants
- Understand the theory of classical and quantum scattering phenomena
- Learn, how to follow the dynamics of chemical reactions experimentally and theoretically

Reference:

1. R. D. Levine, Molecular Reaction Dynamics, Cambridge University Press, NY 2005.
2. J. Steinfield, J. S. Francisco and W. L. Hase, Chemical Kinetics and Dynamics, Prentice Hall Inc., NJ, 1999.

CHE916: Theory of Molecular Spectroscopy (45L+15T Hours)

Coordinators: Prof. U. Lourderaj
u.lourderaj@niser.ac.in

Course Details:

- **Recap**
  Introduction and review of basic quantum mechanics, Molecular symmetry.

- **Rovibronic Hamiltonian - Coordinates and Momenta**
  Euler angles, Axis systems, Rotational and vibrational angular momentum, Normal and internal coordinates, the g matrix, the gF matrix.

- **Rovibronic Wavefunctions**
  Classification of rotational, Vibrational, Rotation-Vibration, and electronic wave functions, Hund's cases.

- **Energy Levels and Interaction**
  Rotation-vibration interactions, Vibronic and rovibronic interactions, Renner-Teller and Jahn-Teller effect, Rydberg states, Spin effects.

- Transition intensities and optical selection rules, Electric – magnetic dipole electric quadrupole transitions, Multiphoton processes and Raman effect.

- **Advanced topics**
  Spectroscopy at high energies, Intramolecular vibrational energy redistribution (IVR), Wave-packet approach to spectroscopy.

Course Outcomes:

- Separate the molecular motion into translations, rotations, and vibrations components
- Transform between internal and normal mode coordinates
- Understand the rovibronic spectroscopy of molecules
- Understand multiphoton processes and their application in modern spectroscopy

Reference:

1. P. R. Bunker and P. Jensen, Molecular Symmetry and Spectroscopy, NRC Research Press, Ottawa.
2. J. D. Graybeal, Molecular Spectroscopy, Mcgraw-Hill.
3. P. F. Bernath, Spectra of Atoms and Molecules, Oxford University press, NY, 1995.
4. E. B. Wilson, J. C. Decius and P. C. Cross, Molecular Vibrations: The Theory of Infrared and Raman Vibrational Spectra, Dover, NY, 1955.

CHE918: Catalysis-Reaction Mechanisms and Applications ((45L+15T Hours)

Coordinators: Prof. C. Gunanathan
gunanathan@niser.ac.in

Course Details:

- **Introduction to Catalysis**
  Fundamental concepts.

- **Survey of Ligands**
  Characteristics of the transition-metal in the complexes; Elementary steps.

- **Reaction Mechanisms and Applications**
  Carbonylation, Hydroformylation, Hydrogenation, metathesis reactions, Oxidation reactions, Isomerization reactions, Cross- Coupling reactions, and C–H functionalization reactions.

- Examples of synthetic and industrial applications.

Course Outcomes:

- Understanding the principles of catalysis.
- Key concepts of various elementary steps which are important in catalytic cycles.
- Understanding the development of various catalysts in many important catalytic reactions
- Implications and applications of catalysis in industry and academia

Reference:

1. The Organometallic Chemistry of the Transition Metals. R. H. Crabtree, John Wiley & Sons, 2005.
2. Industrial Catalysis. J. Hagen, Wiley-VCH, 2006.
3. Homogeneous Catalysis. P. W. N. M. van Leeuwen, Kluwer Academic Publishers, 2004.
4. Homogeneous Catalysis. S. Bhaduri, D. Mukesh, John Wiley & Sons, 2000.
5. Metal-Catalyzed Cross-Coupling Reactions A. De Meijere, F. Diederich (Eds.), 2004.
6. Catalysts for Fine Chemical Synthesis. S. M. Roberts, G. Poignant, John Wiley & Sons, 2002.
7. Catalysis of Organic Reactions, S.R. Schmidt, CRC press, 2007.

CHE919: Advanced Main Group Chemistry (45L+15T Hours)

Coordinators: Prof. Sharanappa Nembenna
snembenna@niser.ac.in

Course Details:

- Direct Bonds Between Metal Atoms: Mg and Ca compounds with metal-metal bond
- Multiple bonded group 13, 14 and 15 elements: Synthesis, reactivity and bonding.
- NHC stabilized low oxidation state main group metal complexes.
- Low Oxidation State Main Group Metal Hydrides: Synthesis and reactivity.
- NHCs Analogues with Low Valent Group 13 and 14 Elements: Synthesis, structure and reactivity studies; (a) Boron (i), Aluminium (i), Gallium (i), Indium (i) and Thallium (i) Heterocycles; (b) Silicon (ii), Germanium (ii), Tin (ii), and Lead (ii) Heterocycles.
- Role of main group compounds in catalysis, organic synthesis and medicinal chemistry
- Inorganic New Materials: Nanomaterials, Polymers and chemical sensors

Course Outcomes:

- Understanding the structure and bonding aspects of metal-metal single or multiple bond of main group elements
- Soluble main group metal hydrides: Synthesis and their reactivity studies
- Group 13 and Group 14 low valent metallacycles: synthesis and reactivity studies
- Application of main group compounds in homogeneous catalysis

Reference:

1. Inorganic Chemistry-Principles of Structure and Reactivity. 4th Edn. Huheey, J. E.; Keiter, E. A.; and Keiter, R. L. Harper-Collins, NY, 1993.
2. Concepts and Models of Inorganic Chemistry. 3rd Edn. Douglas, B.; McDaniel, D.; and Alexander, J. John Wiley, New York. 1993.
3. Chemistry of the Elements. 2nd Edn. Greenwood, N. N.; and Earnshaw, A. Pergamon, Oxford, 1989.
4. Organometallics: A Concise Introduction, C. Elschenbroich and a. Salzer, 3rd Edn. 1999.
5. Inorganic and Organometallic Polymers. Chandrasekhar, V. Springer-Verlag, Heidelberg, 2005

CHE920: Advanced Fluorescence Spectroscopy (45L+15T Hours)

Coordinators: Prof. Moloy Sarkar
msarkar@niser.ac.in

Course Details:

- **Phenomena of Fluorescence and Instrumentation for Fluorescence Spectroscopy**
  Introduction, Jablonski Diagram, Characteristics of Fluorescence Emission, Fluorescence Lifetimes and Quantum Yields, Spectrofluorometers, Light Sources, Monochromators, Optical Filters, Photomultiplier Tubes, Polarizers.

- **Fluorophores**
  Intrinsic or Natural Fluorophores; Fluorescence Enzyme Cofactors, Extrinsic Fluorophores; Protein-Labeling Reagents, Membrane probes, Red and near-infrared (NIR) Dyes, DNA probes, Chemical sensing probes, Viscosity probes, Green fluorescent proteins, Long-lifetime probes, Quantum dots.

- **Life-Time measurements**
  Time-Domain and Frequency-Domain Measurements, Time-Correlated Single-photon Counting, Principle and instrumentation, Alternative Methods for Time-Resolved Measurements; Streak Cameras, Up conversion Methods, Data analysis.

- **Some important Photo-processes**
  Dynamics of Solvent and Spectral Relaxation: Measurement of Time-Resolved Emission Spectra (TRES), Theory for Time-Dependent Solvent Relaxation, Fluorescence Quenching: Theory, Fractional Accessibility to Quenchers, Applications of Quenching to Proteins; Fluorescence Anisotropy: Origin of the Definitions of Polarization and Anisotropy, Measurement of Fluorescence anisotropies, Causes of Depolarization, Biochemical Applications. Energy Transfer: Theory of Energy Transfer for a Donor acceptor pair, Distance Measurements Using Resonance Energy Transfer (RET), Biochemical applications of RET.

- **Multiphoton Excitation**
  Introduction to Multiphoton Excitation, Two-photon Absorption Spectra, Cross Section for Multi-photon Absorption.

- **Single-molecule Detection (SmD)**
  Detectability of Single Molecules, Instrumentation for SMD, Single-Molecule photophysics, Biochemical applications of SMD.

- **Fluorescence Correlation Spectroscopy (FCS)**
  Principles of Fluorescence Correlation Spectroscopy, Theory of FCS, Examples of FCS Experiments.

- **Fluorescence-Lifetime imaging microscopy (FLim)**
  Early Methods for Fluorescence-Lifetime imaging, Laser Scanning TCSpC FLiM, Lifetime imaging of Cellular Biomolecules.

- **Radiative Decay engineering**
  Introduction to Radiative Decay Engineering, Review of Metal Effects on Fluorescence Surface Plasmon-Coupled Emission (SPCE), Applications of Metal-Enhanced Fluorescence, Application of SPCE.

Course Outcomes:

- Describes basic principles and application of fluorescence spectroscopy
- To learn, how fluorescence spectroscopy is used for frequency and time domain studies of important chemical process
- To learn to use fluorescence spectroscopy in biomolecules
- It also introduces fluorescence imaging

Reference:

1. Principles of Fluorescence Spectroscopy, Joseph R. Lakowicz, 3rd Edn., Springer, 2006.
2. Advanced Time-correlated Single Photon Counting Techniques, W. Becker, Springer, 2005.
3. Molecular Fluorescence Principles and Applications, B. Valeur, WILEY-VCH, 2002.
4. Single-Molecule Detection in Solution. Methods and Applications, C. Zander, R. A. Keller, and J. Enderlein, WILEY- VCH, 2001

CHE921: Bio macromolecules (45L+15T Hours)

Coordinators: Dr. C. S. Purohit
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Course Details:

- Buffers (their use in study of biomolecules), pH, pKa of amino acids, D and L amino acid nomenclature.

- Biophysical techniques to purify and study proteins Dialysis, Salting out and precipitation by organic solvents, Ion exchange, Gel filtration, Reversed phase, Affinity chromatography, Ultracentrifugation, Gel electrophoresis.

- **Proteins**
  Protein sequencing by chemical and mass & NMR spectroscopic methods, Use of spectroscopic tools in studying biomolecules. Primary (single letter amino acid codes), Ramachandran plot, Secondary structures like helices, parallel- and antiparallel-sheets, Circular Dichroism of secondary structures, Tertiary (motifs and domains: some important motifs like Rossman fold, helix turn helix, 4 helix bundles, beta barrel), Quaternary structure (Haemoglobin and Myoglobin) and Enzymes.

- **Nucleic acids**
  A, B and Z-DNA structures, Method of replication, Sequencing of nucleic acids (Chemical, dideoxy and fluorescence), Transcription, Translation, Genetic code, Genomes, Genes, overexpression of recombinant proteins, Mutagenesis (random and site directed); Polymerase Chain Reaction (PCR).

- Carbohydrates and glycoproteins, Proteoglycans, Membranes and lipids, Bacterial cell wall synthesis and mechanism of some important antibiotics like Penicillin, Antibiotic resistance.

- **Metabolism**
  Photosynthesis, Calvins cycle, Glycolysis, Krebs cycle, Electron transport, Cofactors.

Course Outcomes:

- Basic understanding of biomolecules with respect to their structure
- Structure and function relation of biologically important molecules
- In-depth understanding of various biological processes such as DNA replication, protein synthesis

Reference:

1. Voet, D; Voet, J. G; Pratt, C. W., Fundamentals of Biochemistry: Life at the Molecular Level, 2nd Edn.,2006
2. Berg J. M, Tymoczko J. L. and Stryer L., Biochemistry, 6th Edn.,2007.
3. Creighton, T. E., Proteins: Structure and Molecular Properties, 2nd Edn., 1993.
4. Lewin B., Genes IX, 2008
5. Branden C and Tooze J., Introduction to Protein Structure, 2nd Edn., 1999.
6. Fersht A., Structure and Mechanism in Protein Science: A Guide to Enzyme Catalysis and Protein Folding, 1999.

CHE922: Advanced Heterocyclic Chemistry (45L+15T Hours)

Coordinators: Dr. N. K. Sharma
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Course Details:

- Heterocyclic Chemistry; Introduction to heterocycles: Nomenclature, Spectral characteristics, Reactivity and Aromaticity.
- Synthesis and reactivity of three and four membered heterocycles e.g., Aziridine, Azirine, Azetidine, Oxiranes, Thiarines, Oxetenes and Thietanes.
- Synthesis and reactivity of five membered rings with two heteroatoms,Pyrazole, Imidazole, Oxazole, Thiazole, Isothiazole and Benzofused analogs; Benzo-fused five membered heterocycles with one heteroatom, e.g., Indole, Benzofuran, Benzothiophene.
- Synthesis and reactivity of benzofused six membered rings with one, two and three heteroatoms: Benzopyrans, Quinolines, Isoquinoline, Quinoxazaline, Acridine, Phenoxazine, Phenothiazine, Benzotriazine, Pteridines.
- Synthesis and reactivity of seven and large membered heterocycles Azepines, Oxepines, Thiepines; Spiro-heterocycles; Bicyclic compounds containing one or more heteroatoms

Course Outcomes:

- Introduction of Heterocyclic Chemistry: Nomenclature, spectral characteristics, reactivity and aromaticity of heterocycles (three- and four-membered)
- Synthesis and reactivity of five-membered rings, benzo-fused six-membered rings with one, two and three heteroatoms, seven and large membered
- Recent methods of C−H functionalization/activations of heterocyclic derivatives
- Beneficial to synthesized therapeutic drugs

Reference:

1. Carey, F. A. & Sundberg, R. J. Advanced Organic Chemistry, Partsa & B., Plenum: U.S., 2004
2. Thomas. L. Gilchrist, Heterocyclic Chemistry, (3rd Edn.), 1997.
3. Joules, J.A; Mills, K.; Smith, G.F. Heterocyclic Chemistry, 3rd Edn.
4. Advances in Heterocyclic Chemistry, Book Series Elsevier Edited by Alan Katritzky.
5. Branden C and Tooze J., Introduction to Protein Structure, 2nd Edn., 1999.

CHE923: Statistical Mechanics (45L+15T Hours)

Coordinators: Dr. B. L. Bhargava
bhargava@niser.ac.in

Course Details:

- Basic assumptions, Concept of microscopic and macroscopic states, Ensembles and averages; Calculation of distribution functions in canonical ensemble and the canonical partition function; Relations between the canonical partition function and thermodynamic functions; Calculations in other ensembles like microcanonical and grand canonical ensembles. Calculations of fluctuations and equivalence of ensembles.

- Calculations of partition functions and thermodynamic properties for ideal systems of monatomic and diatomic molecules. Calculations of fluctuations and equivalence of ensembles

- Calculation of heat capacity of solids, Einstein and Debye theories, Study of chemical equilibrium in terms of partition functions.

- **Quantum Statistics**
  Maxwell-Boltzmann, Bose-Einstein, and Fermi-Dirac statistics. Systems of Fermions and Bosons in weak and strong degenerate limits.

- **Classical Statistical Mechanics**
  Partition functions as integrals over phase space coordinates, Systems of interacting particles, imperfect gases, concept of radial distribution functions of liquids and applications to ionic solutions using Debye-Huckel theory.

- **Non-equilibrium Statistical Mechanics**
  Onsager regression hypothesis and fluctuation-dissipation theorem, Calculations of transport coefficients like Diffusion and Conductivity.

Course Outcomes:

- Understanding the concepts of ensembles, energy partition and probability distribution
- Learning of classical and quantum statistical mechanics
- Application of statistical mechanics to study the thermodynamic properties of simple gases and solids.

Reference:

1. Physical Chemistry: A Molecular Approach, D. A. McQuarrie and J. D. Simon, Viva Books, New Delhi, 1998.
2. Statistical Mechanics, D.A. McQuarrie, University Science Books, 2nd Edn., 2000.
3. Introduction to Modern Statistical Mechanics, D. Chandler, Oxford Univ. Press, 1987.
4. Statistical Thermodynamics of Non-Equilibrium Processes, J. Kaizer, Springer, 1st Edn., 1987.
5. Statistical Physics II: Non-Equilibrium Statistical Mechanics, R. Kubo, M. Toda and N. Hashitsume, Springer, 2003.

CHE924: Frontiers in Organic Synthesis (45L+15T Hours)

Coordinators: Dr. S. Peruncheralathan
peru@niser.ac.in

Course Details:

- Developing facets of organic synthesis.

- **Domino Reactions**
  History, Definition, Classifications, Biological systems, Enantioselective reactions and Application in total synthesis.

- **Non-activated C–H Functionalization**
  Mode of activation, Metal and Organocatalysts, Traceless organic synthesis, Decarboxylative cross-coupling reactions, Remote C-H functionalization, Recent examples

- **Protecting Group Free Total Synthesis**
  Historical context, Protection and Deprotection, Chemoselectivity, Recent advances in protecting groups free total synthesis

- **Recent Applications**
  Click Chemistry, Mechanochemistry, Photocatalysis

Course Outcomes:

- To learn frontier research in chemical synthesis
- To understand applications of cutting edge methodology used in synthesizing target molecules
- To learn Greener Chemical Synthesis

Reference:

1. L. F. Tietze, G. Brasche, K. Gericke, “Domino Reactions in Organic Synthesis” 1st Edition, Wiley-VCH, 2006.
2. L. F. Tietze (Editor), “Domino Reactions: Concepts for Efficient Organic Synthesis” 1st Edition, Wiley-VCH, 2014.
3. G. Dyker (Editor) “Handbook of C-H Transformations: Applications in Organic Synthesis-Two volumes” 1st Edition, Wiley-VCH, 2005.
4. Journal Articles and Reviews