INTEGRATED M.Sc. (13) (CHEMICAL SCIENCES)

Programme Code: CHEM13

Programme Outcome:

- Ability to learn and engage in emerging areas of Chemical Sciences
- Ability to collaborate and work in interdisciplinary areas of science where chemistry knowledge is required.
- Ability to pursue a career in Chemical Research
- Human resource with knowledge base in theoretical and experimental Chemistry
- Ability to work on societal problems involving Chemistry
- Ability to apply the basic concepts and principles of Chemistry in solving real life problems

DETAILED COURSE STRUCTURE

CORE COURSES					
Year/Semester	**Course Code**	**Name of the Course**	**Hours**		**Credits**
			L	**T / P**	
1 Year /Semester-I	CHE101	Chemistry I	30	15	3
	CHE141	Chemistry Laboratory		60 (P)	2
1 Year /Semester-II	CHE102	Chemistry II	30	15	3
2 Year /Semester III (20 Credits)	CHE201	Basic Inorganic Chemistry	45	15	4
	CHE203	Reaction Mechanism in Organic Chemistry	45	15	4
	CHE205	Mathematical Methods for Chemists	45	15	4
	CHE241	Inorganic Chemistry Laboratory		120(P)	4
	HSS###	Elective from SHSS	30		2
	HSS###	Elective from SHSS	30		2
2 Year /Semester III (20 Credits)	CHE202	Reagents in Organic Synthesis	45	15	4
	CHE204	Main Group and Organometallic Chemistry	45	15	4
	CHE206	Thermodynamics and Electrochemistry	45	15	4
	CHE242	Organic Chemistry Laboratory		120(P)	4
	HSS###	Elective from SHSS	30		2
	HSS###	Elective from SHSS	30		2
3 Year /Semester V (20 Credits)	CHE301	Physical Organic Chemistry	42	14	4
	CHE303	Physical Methods in Chemistry I	42	14	4
	CHE305	Molecular Quantum Mechanics	42	14	4
	CHE341	Physical Chemistry Laboratory		120(P)	4

3 Year /Semester V (20 Credits)	**	Out of Stream Elective 1			4
3 Year /Semester VI (20 Credits)	CHE302	Coordination Chemistry	45	15	4
	CHE304	Molecular Spectroscopy and Group Theory	45	15	4
	CHE306	Physical Methods in Chemistry II	45	15	4
	CHE342	Computational Chemistry Laboratory		120(P)	4
	**	Out of Stream Elective 2			4
4 Year /Semester VII (20 Credits)	CHE401	Chemistry of Heterocycles and Natural Products	45	15	4
	CHE403	Chemical Rate Processes	45	15	4
	CHE498	Chemistry Project			8
	**	Out of Stream Elective 3	60		4
4 Year /Semester VIII (20 Credits)	CHE499	Chemistry Project			8
	*	Elective - I	45	15	4
	*	Elective - II	45	15	4
	**	Out of Stream Elective 4	45	15	4
5 Year /Semester IX (20 Credits)	CHE598	Chemistry Project	45	15	12
	*	Elective - III	45	15	4
	***	Elective – IV (In/Out of stream 5)	45	15	4
5 Year /Semester X (20 Credits)	CHE599	Chemistry Dissertation	45	15	12
	*	Elective - V	45	15	4
	***	Elective - VI (In/Out of stream 6)	45	15	4

Course Structure for a Minor in Chemistry

To earn a minor, students have to take courses with a minimum of 20 credits in Chemistry (from courses offered by SCS, second year onwards). The students must take the following courses.

Sl. No.	Course Code	Name of the Course	Hours		Credits
			L	T	
1	CHE201	Basic Inorganic Chemistry	45	15	4
2	CHE203	Reaction Mechanism in Organic Chemistry	45	15	4
3	CHE206	Thermodynamics and Electrochemistry	45	15	4
4	CHE302	Coordination Chemistry	45	15	4
5	CHE303	Physical Methods in Chemistry - I	45	15	4
Total			300		20

** is in-stream elective;*
*** is out-of-stream elective*
**** electives I-V have to be from the list of elective courses*
L = Class hours, P = Lab hours, T =Tutorial hours/week

SYLLABUS FOR ELECTIVE COURSES

ELECTIVE COURSES					
Sl. No	**Course Code**	**Name of the Course**	**Hours**		**Credits**
			L	**T**	
1	CHE351	Photochemistry	45	15	4
2	CHE352	Pharmaceutical Chemistry	45	15	4
3	CHE353	Classics in Molecules	45	15	4
4	CHE551	Molecular Modeling	45	15	4
5	CHE552	Solid State Chemistry	45	15	4
6	CHE554	Crystallography	45	15	4
7	CHE555	Principles of Drug Action	45	15	4
8	CHE556	Advanced Bio-inorganic Chemistry	45	15	4
9	CHE557	Nuclear Magnetic Resonance	45	15	4
10	CHE558	Advanced Functional Materials	45	15	4
11	CHE559	Supramolecular Chemistry	45	15	4
12	CHE560	Chemistry of Nanomaterials	45	15	4
13	CHE561	Advanced Bio-organic Chemistry	45	15	4
14	CHE562	Polymer Chemistry	45	15	4
15	CHE563	Molecular Reaction Dynamics	45	15	4
16	CHE564	Theory of Molecular Spectroscopy	45	15	4
17	CHE565	Advanced Organic Chemistry	45	15	4
18	CHE566	Catalysis: Reaction Mechanisms and Applications	45	15	4
19	CHE567	Advanced Main Group Chemistry	45	15	4
20	CHE568	Advanced Fluorescence Spectroscopy	45	15	4
22	CHE570	Advanced Heterocyclic Chemistry	45	15	4
21	CHE569	Bio macromolecules	45	15	4

23	CHE571	Statistical Mechanics	45	15	4
24	CHE572	Frontiers in Organic Synthesis	45	15	4
25	CHE573	Chemical Binding	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 Courses		
Name of the Course	**Course Coordinator Name**	**Email ID**
Chemistry I	Prof. Moloy Sarkar	spraka@hbni.ac.in
Chemistry II	Dr. Bidraha Bagh	bidraha@niser.ac.in
Basic Inorganic Chemistry	Dr. Deepak Samanta	dsamanta@niser.ac.in
Reaction Mechanism in Organic Chemistry	Dr. C. S. Purohit	purohit@niser.ac.in
Mathematical Methods for Chemists	Dr. B. L. Bhargava	bhargava@niser.ac.in
Reagents in Organic Synthesis	Dr. Nagendra K. Sharma	nagendra@niser.ac.in
Main Group and Organometallic Chemistry	Prof. Sharanappa Nembenna	snembenna@niser.ac.in
Thermodynamics and Electrochemistry	Dr. Partha Maity	pmaity@niser.ac.in
Physical Organic Chemistry	Prof. Prasenjit Mal	pmal@niser.ac.in
Physical Methods in Chemistry I	Dr. Bishnu P. Biswal	bp.biswal@niser.ac.in
Molecular Quantum Mechanics	Prof. Himansu S. Biswal	himansu@niser.ac.in
Coordination Chemistry	Dr. Deepak Samanta	dsamanta@niser.ac.in
Molecular Spectroscopy and Group Theory	Prof. Subhadip Ghosh	sghosh@niser.ac.in
Physical Methods in Chemistry II	Prof. A. Srinivasan	srini@niser.ac.in
Chemistry of Heterocycles and Natural Products	Prof. C. Gunanathan	gunanathan@niser.ac.in
Chemical Rate Processes	Prof. Moloy Sarkar	msarkar@niser.ac.in

ELECTIVE COURSES COORDINATOR

Elective Courses		
Name of the Course	**Course Coordinator Name**	**Email ID**
Photochemistry	Dr S. Peruncheralathan	peru@niser.ac.in
Pharmaceutical Chemistry	Dr. S. Peruncheralathan	peru@niser.ac.in
Classics in Molecules	Dr. S. Peruncheralathan	peru@niser.ac.in
Molecular Modeling	Prof. U. Lourderaj	u.lourderaj@niser.ac.in
Solid State Chemistry	Prof. J. N. Behera	jnbehera@niser.ac.in
Crystallography	Prof. J. N. Behera	jnbehera@niser.ac.in
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	Prof. U. Lourderaj	u.lourderaj@niser.ac.in
Advanced Organic Chemistry	Dr. Rajkumar Misra	rajkumarmisra@niser.ac.in
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
Advanced Heterocyclic Chemistry	Dr. N. K. Sharma	nagendra@niser.ac.in
Bio macromolecules	Dr. C. S. Purohit	purohit@niser.ac.in
Statistical Mechanics	Dr. B. L. Bhargava	bhargava@niser.ac.in
Frontiers in Organic Synthesis	Dr. S. Peruncheralathan	peru@niser.ac.in
Chemical Binding	Dr. Arindam Ghosh	aringh@niser.ac.in

LABORATORY EXPERIMENTS COURSES COORDINATOR

Laboratory Courses		
Name of the Course	**Course Coordinator Name**	**Email ID**
Chemistry Laboratory	Prof. Subhadip Ghosh	sghosh@niser.ac.in
Inorganic Chemistry Laboratory	Dr. Bidraha Bagh	bidraha@niser.ac.in
Organic Chemistry Laboratory	Dr. S. Peruncheralathan	peru@niser.ac.in
Physical Chemistry Laboratory	Prof. Himansu S. Biswal	himansu@niser.ac.in
Computational Chemistry Laboratory	Prof. U. Lourderaj	u.lourderaj@niser.ac.in

DETAILED SYLLABUS CORE COURSES

C101: Chemistry I (CHE-101-C) (30 L+15T)

Coordinators: Prof. Moloy Sarkar
spraka@hbni.ac.in

Course Details:

- **Thermodynamics and Chemical equilibrium**
  Laws of thermodynamics; Thermochemistry; Joule-Thomson Effect; Entropy, Helmholtz and Gibbs free energies, Maxwell Relations, Partial molar quantities, Chemical potential, Gibbs- Duhem equation. Equilibrium constant and its relation with free energy changes, Variation of chemical equilibrium constant with temperature and pressure, van't Hoff equation, Applications of Gibbs-Helmholtz equation.

- **Elementary Chemical Kinetics**
  Rate laws for first, second and third order reactions, Reversible, parallel and consecutive reactions, Steady state approximation, Enzyme kinetics (Michaelis-Menten equation).

- **Rate Theories and Dynamics**
  Temperature dependence of the rates of chemical reactions, Collision theory, Qualitative concepts of transition state theory, Introduction to reaction dynamics.

- **Atomic and Molecular Structure**
  Introduction to quantum mechanics: Particle in a box, Atomic structure: Hydrogen atom, concept of atomic orbitals and wave functions, Many electron atoms, Spin and Pauli principle. Molecules: Bonding in homo and heteronuclear diatomic molecules]

- **Spectroscopy**
  Interaction of light with matter, Electronic spectroscopy, Beer- Lambert's law, Fluorescence, Phosphorescence, Rotation and vibrational spectroscopy, Introduction to Nuclear Magnetic Resonance (NMR), Application of spectroscopy to Biomolecules.

Course Outcomes:

- The basics of atomic and molecular structure; introduction to spectroscopy
- Thermodynamics of different chemical processes
- Kinetics of chemical reactions

References:

1. Physical Chemistry, I. Levine, Tata Mcgraw Hill, 5th Edn., 2007.
2. Physical Chemistry: A Molecular Approach, D. A. McQuarrie and J. D. Simon, University Science Books, 1997.
3. Physical Chemistry, G. M. Barrow, Mcgraw Hill, 5th Edn., 2007.
4. Chemical Kinetics, K. J. Laidler, 3rd Edn., Harper and Row, 1987.

C102: Chemistry II (CHE-102-C) (30 L+15T)

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

Course Details:

- Structure of simple inorganic molecules; VSEPR theory; Coordination complexes; Brief description of VBT, CFT and MO theory; Distortion in octahedral complexes.

- Organometallic chemistry; Metal carbonyls; Metal nitrosyls; 18 electron rule; Ferrocene and its basic reactions; Catalysis of organometallic complexes; Hydrogenation and other industrially important reactions.

- Chemistry of biological systems; Haemoglobin, Myoglobin and Heme containing systems.

- Structure of organic molecules (Lewis structures, acid-Base, HSAB principles, Hybridization, Resonance, Hyper- conjugation, Aromaticity, Functional groups, Nomenclature, Isomerism).

- Conformational analysis of acyclic and cyclic systems; Molecular chirality; Cohn- Ingold-Prelog R-S notational system; Optical activity; Chiral induction; Importance of chirality in chemical biology.

Course Outcomes:

- Apply the fundamental principles of measurement, matter, atomic theory, chemical periodicity, chemical bonding, general chemical reactivity and solution chemistry to subsequent courses in Science, Engineering and Technology
- Students will be able to explain why Chemistry is an integral activity for addressing social, economic, and environmental problems
- Students will be able to explore new areas of research in both Chemistry and allied fields of Science and Technology after understanding the basic concepts in Chemistry

References:

1. S. H. Pine, Organic Chemistry, 5th Edn. Tata Mcgraw Hill Book Co., 2007.
2. T. W. G. Solomons, C. B. Fryhle, Organic Chemistry, 8th Edn. Wiley, 2007.
3. T. W. G. Solomons, C. B. Fryhle, R. G. Johnson, Study guide and Solutions Manual to accompany: Organic Chemistry, 8th Edn. John Wiley & Sons, 2005.
4. J. Karty, The Nuts and Bolts of Organic Chemistry: A Student's Guide to Success, Pearson, 2008.
5. R. J. Morrison and R. N. Boyd, Organic Chemistry, 6th Edn. Prentice Hall, 2007.
6. J. E. Huheey, E.A. Keiter, R. L. Keiter, O. K. Medhi, Inorganic Chemistry: Principles of Structure and Reactivity, 4th Edn. Pearson, 2007.
7. P. Atkins, T. Overton, J. Rourke, M. Weller, F. Armstrong, Shriver & Atkins Inorganic Chemistry, 4th Edn. Oxford, 2009.
8. B. D. Gupta, A. J. Elias, Basic Organometallic Chemistry: Concepts, Syntheses and Applications, Universities press, 2010.

C201: Basic Inorganic Chemistry (CHE-201-C) (45 L+15T)

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

Course Details:

- **Basic Solid-State Chemistry**
  The ionic bond, Lattice Energy, Size effects, Covalent character in predominantly ionic bonds, Structures of complex solids, Imperfections in Crystals, Conductivity in ionic solids, Solids held together by Covalent bonding.

- **Molecular Structure and Chemical Forces**
  Molecular symmetry, Point groups and introduction to Character Tables; Types of chemical forces: Covalent bonding, Hydrogen bonding, Effects of chemical forces.

- **Basic Main Group Chemistry**
  First and second row anomalies, Use of p orbitals in π-bonding, Use (or not) of d orbitals by non-metals, Reactivity of d orbital participation, Periodic anomalies of the non-metals and post-transition metals, Chains catenation, Rings, Cages, Boron cage compounds.

- **Coordination Chemistry**
  Structure, Isomerism, Stability, Reactions, Kinetics and Mechanisms: Coordination number 1 - 8, Higher coordination number, Types of isomerism, Thermodynamic stability, Chelate Effect, Substitution reactions in Square planar complexes, Thermodynamic and Kinetic stability, Kinetics of Octahedral substitution and Mechanisms of redox reactions.

- **Oxidation and Reduction**
  Reduction potentials; Redox half reactions; Trends in standard potentials, Electrochemical series, the Nernst equation, Redox stability in water; Representation of electrode potential data diagrammatically. Latimer–Frost Diagrams, Chemical extraction of elements through oxidation, reduction and electrochemical extraction.

- **Introduction to f-block Elements**
  Special features of f-block elements, Lanthanide contraction, Coordination number, structures, and simple reactions.]

- **Nuclear Chemistry**
  Nuclear reactions and their characteristics, Radioactivity, Detecting and measuring radioactivity, Radioactive decay rates, Nuclear stability, Energy changes during nuclear reactions, Nuclear fission and fusion, Nuclear transmutation, Biological effects of radiation; Some applications of nuclear Chemistry: Dating with radioisotopes, Medical uses therapeutic and imaging procedures.

Course Outcomes:

- To understand basic facts and concepts in Chemistry while retaining the exciting aspects of Chemistry so as to develop interest in the study of Chemistry as a discipline.
- To develop the ability to apply the principles of Chemistry.
- To appreciate the achievements in Chemistry and to know the role of Chemistry in nature and in society.
- To develop problem solving skills.

- To be familiarized with the emerging areas of Chemistry and their applications in various spheres of Chemical Sciences and to apprise the students of its relevance in future studies.
- To be exposed to the different processes used in industries and their applications

References:

1. Chemistry of the Elements, N. N. Greenwood and A. Earnshaw, 2nd Edn., Elsevier, 2005.
2. Chemistry, J. McMurry, R. C. Fay, 4th Edn., Pearson Education, 2005.
3. Group Theory and Chemistry, D. M. Bishop, Dover Publications, New York, 1973.
4. Chemical Applications of Group Theory, F. A. Cotton, John Wiley and Sons, 2003.
5. Inorganic Chemistry- Principles of Structure and Reactivity, J. E. Huheey, E. A. Keiter, R. L. Keiterand, O. K. Medhi, Pearson Education, 2007.
6. Concise Inorganic Chemistry, J. D. Lee, 4th Edn., ELBS, 1991.
7. Advanced Inorganic Chemistry, F. A. Cotton, C. A. Murillo, and M. Bochmann, Wiley Inter Science, 2001.
8. Inorganic Chemistry, D. F. Shriver and P. W. Atkins, Oxford University, 1999.
9. Molecular Symmetry and Group Theory: A Programmed Introduction to Chemical Applications, A. Vincent, John Wiley, 2001.

C203: Reaction Mechanisms in Organic Chemistry (CHE-203-C) (45 L+15T)

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

Course Details:

- **Structural effects on Stability and Reactivity**
  Thermodynamic Stability; Chemical Kinetics; Thermodynamic Stability vs Reaction Rates; Electronic Substituent Effects on Reaction intermediates; Kinetic Isotope Effects; Linear Free-Energy relationships for substituent effects; Catalysis; Solvent effects; Highly strained molecules.

- **Nucleophilic Substitution Reactions**
  Nucleophiles, Electrophiles and Leaving groups; Mechanisms for nucleophilic substitution; Kinetic and stereochemical analysis; Substituent effects on reactivity; SN2 Reaction vs SN1 Reaction; Neighboring group participation; SNi Reactions; Preparative useful SN2 Reactions; Carbocationic rearrangements. [10]

- **Addition Reactions**
  The Concept of cis- and trans-addition; Electrophilic addition of alkenes; Selected examples – Hydrohalogenation, Halogenations, Hydration, Epoxidation, Dihydroxylation, Sulfenylation, Halolactonization, Metal ions, Hydroboration, Cyclopropanation; Electrophilic addition of alkynes and allenes; Vocabulary of Chemoselectivity, Diastereoselectivity, Enantioselectivity, Stereospecificity, Stereoconvergence; Asymmetric Catalysis – Sharpless Oxidations of allylic alcohols and dihydroxylation; Noyori hydrogenation.

- **Elimination Reactions**
  Concepts of elimination reactions; Mechanism of E2, E1 and E-CB reactions; Regioselectivity and Stereoselectivity of elimination reactions; The competition between elimination and nucleophilic substitution reactions; Substrate effects, Base effects, Stereoelectronic Effect; Heck Reaction, Carbene, Nitrene.

- **Aromatic Substitution**
  Aromaticity; Annulenes; Electrophilic aromatic substitution reactions; Substituent effects on reactivity; Nucleophilic aromatic substitution; Ortho metallation; Cross-coupling reactions.

Course Outcomes:

- Introduction of basic organic reactions (Substitutions, Additions & Eliminations) and writing organic reaction mechanisms.
- Reactivity of unsaturated hydrocarbons (alkene, alkyne and aromatics).
- Understanding the role of substitutions to influence the rate of reactions.
- Stereochemistry in organic chemistry: Chemoselectivity, Diastereoselectivity, Enantioselectivity, Stereospecificity, Stereoconvergence.
- Introduction of asymmetric synthesis with and without asymmetric catalysts.

References:

1. F. A. Carey, R. J. Sundberg "Advanced Organic Chemistry Part A and 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 Edn., Wiley- VCH, 2007.
5. E. V. Anslyn, D. A. Dougherty "Modern Physical Organic Chemistry" California University Science Books, 2006.

C205: Mathematical Methods for Chemists (CHE-205-C) (45 L+15T)

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

Course Details:

- **Matrix Algebra**
  Matrices, Determinants, Matrix rank, Orthogonal and unitary transformations, Eigenvalues and eigenvectors, Diagonalization of matrices, Spectral theorem, and few applications.

- **Vectors and Tensors**
  Introduction to vectors; Vector operations; Coordinate system transformation; Covariant and contravariant vector components and few applications; Vector spaces, Inner products, Linear independence, Bases; Brief introduction to tensors, Tensor algebra.

- **Ordinary Differential Equations**
  Linear first and second order ODEs, Homogeneous and inhomogeneous ODEs with constant coefficients, System of linear ODEs, Power series solution of differential equations and special functions.

- **Fourier Series and Integral Transforms**
  Fourier series and transform, properties and theorems, Multi-dimensional FT, Complex FT, Discrete and digital FT and few applications. Brief introduction to Laplace transform, Inverse Laplace transform, convergence of Laplace integral and few applications.

- **Data and Error Analysis**
  Interpolation and extrapolation, Errors in physical systems, Random errors in measurements, Uncertainties as probabilities, Error propagation, Normal distribution, Curve fitting.

Course Outcomes:

- Introduce the standard mathematical techniques that are typically used by Chemists.
- To learn how to apply mathematics in Chemical Research.
- To learn how to use Fourier transforms in Spectroscopy.
- The course, mostly differential equations, is useful to learn Quantum Chemistry and Chemical Kinetics.

References:

1. Maths for Chemists: G. Doggett, M. Cockett, E. Abel: RSC (Tutorial Chemistry Texts), 2012.
2. Basic Mathematics for Chemists: P. Tebbutt: Wiley-Blackwell, 1998.
3. Mathematical Methods in the Physical Sciences: M. L. Boas, Wiley, 2005.
4. A student’s guide to vectors and tensors, D. Fleisch, Cambridge Univ. Press, 2008.
5. Measurements and their uncertainties, I. G. Hughes and Thomas P. A. Hase, Oxford Univ. Press, 2010.
6. Mathematical Methods for Physicists: Arfken and Weber, Elsevier Academic Press, 2005.
7. The Fourier transform and its applications, 3rd Edn, R. N. Bracewell, McGraw Hill Intl. Edn.,2000.

C202: Reagents in Organic Syntheses (CHE-202-C) (30 L+15T)

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

Course Details:

- **Chemistry of Carbonyl Groups**
  Nucleophilic addition to Carbonyl groups; Nucleophilic substitution at Carbonyl groups and with complete removal of Carbonyl oxygen; Carbanions and Enolisation; Building organic molecules from Carbonyl compounds (well-known Name Reactions); Nitrogen, Phosphorus and Sulfur Ylides; Michael addition. [20]

- **Oxidation Reactions**
  Transition metal-based oxidation reagents; DMSO- based oxidation reactions; Other oxidation reagents; Oxidation of functional groups; Oxidative cleavage of C=C bonds and glycols; Ozonolysis; Barton Reaction; Oxidations at unfunctionalized C-H Bonds.

- **Reduction Reactions**
  Reduction of Carbonyl groups: Conformational effects; Stereochemistry of hydride reduction reactions – Aluminium hydride and Borohydride reducing agents; Hydride reductions of functional groups; Dissolving metal reductions; Other reduction methods; Corey-Bakshi-Shibaki reduction.

- **Retrosynthesis**
  Principles and applications; Target-oriented and diversity- oriented organic synthesis; Selected examples. [7]

Course Outcomes:

- Design the chemical reactions based on various metals and non-metal reagents.
- Application of the reagents in organic synthesis.
- Design the synthesis of unknown target molecules.

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 Edn., Wiley- VCH, 2007.
5. E. J. Corey, X.-M. Cheng "The Logic of Chemical Synthesis" Wiley- Interscience, 1995.
6. T. Hudlicky, J. W. Reed "The Way of Synthesis: Evolution of Design and Methods for natural products" Wiley-VCH, 2007.

C204: Main Group and Organometallic Chemistry (CHE-204-C) (45 L+15T)

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

Course Details:

- Basic Characterization techniques of main-group and organometallic compounds (NMR, Mass, IR). [5]

- **Representative chemistry of main group elements**

  - Organometallic chemistry of lithium and magnesium: synthesis, Structures and reactivity**.**

  - Chemistry of Boron: Boranes, bonding in Boranes, Topology of Boranes, synthesis and reactivity, Carboranes and metallacarboranes. New Lewis acids based on Boron; Polymer-supported Lewis acids.

  - Chemistry of Aluminum: Aluminum alkyls. Use of aluminum alkyls in polymerization of olefins.

  - C60 and Carbon nanotubes: discovery, preparation and selected reactions.

  - Chemistry of Silicon: Organosilicon compounds, Silicates and aluminosilicates

- **Unusual compounds of main group elements**
  - Chemistry of multiple bonding: Multiple bonding in heavier main-group elements. Unusual compound of main group elements: Si=Si, Si≡Si, P=P double bond, Bi=Bi double bond. Synthesis, structure and reactivity; Controversies.

  - Chemistry of low valent compounds: Synthesis, structure and bonding models and reactivity examples of Al (i), Si (ii) low valent compounds.

  - Low oxidation state main group metal hydrides: synthesis and reactivity studies.

  - Inorganic rings and polymers. Cyclo and hetero cyclophosphazenes and the polymers derived from them. Polysilanes. Borazine and Boron Nitride.

  - Chemistry of halogens and noble gases – recent trends. CFCs and ozone layer.

- **Organometallic Chemistry**

  - σ-bonded ligands: Metal alkyls, aryls and hydrides. Stability, Preparation and reactivity.

  - Metal-carbonyls / Metal-phosphines / Metalnitrosyls / Metal iso-cyanide: Structures, reactivity and bonding. Metalcarbenes, Metal-carbynes, Fischer carbenes, Schrock carbenes, N-heterocyclic carbenes, Olefin metathesis

  - π-bonded ligands: Metal-olefins, Metal alkynes, Metal-dienes, Metal-Cp Metal-Cp* complexes: Synthesis, structure, bonding and reactivity

  - Applications of organometallics in organic synthesis: C–C bond coupling reactions (Heck, Sonogoshira, Suzuki etc.). C–N bond coupling reactions. Reduction reactions using transition metal hydrides; Asymmetric hydrogenation.

Course Outcomes:

- Learn the characterization of organometallic compounds.
- Learn the synthesis, structure and application of organometallics of Li, Mg, B, Al and Si elements.
- Understand the synthesis, structure and bonding aspects of selected examples of unusual main group compounds.
- Organometallics of transition metal Chemistry and its application in catalysis.

References:

1. Organometallics: A Concise Introduction, C. Elschenbroich and A. Salzer, 3rd Edn. 1999.
2. Chemistry of the Elements, N. N. Greenwood and A. Earnshaw, 2nd Edn., Elsevier, 2005.
3. Modern Inorganic Chemistry, W. L. Jolly, Mcgraw Hill, New York, 2nd Edn., 1991.
4. Concepts and Models of Inorganic Chemistry, B. Douglas, D. McDaniel and J. Alexander, John Wiley, New York, 3rd Edn., 1993.
5. Organometallic Chemistry of the Transition Metals, R. H. Crabtree, Wiley, New York, 1988.

C206: Thermodynamics and Electrochemistry (CHE-206-C)) (45 L+15T)

Coordinators: Dr. Partha Maity
pmaity@niser.ac.in

Course Details:

- **Recap**
  Review of thermodynamics and chemical equilibrium. Phase equilibrium: Multicomponent systems, Ideal solution, Vapor–liquid equilibrium, Raoult's law, Henry's law, colligative properties.

- **Surfaces**
  Thermodynamics of surfaces and interfaces, Surface tension, Vapour pressure; Surface films on liquids, Gibb's adsorption equation; Adsorption of gases on solids: Freundlich, Langmuir and BET adsorption isotherms; Determination of surface areas; Colloids.

- **Electrochemistry**
  Review of thermodynamics and chemical equilibrium. Phase equilibrium: Multicomponent systems, Ideal solution, Vapor–liquid equilibrium, Raoult's law, Henry's law, colligative properties.

- Electrochemical Cells and Electromotive Force (EMF), Thermodynamics of cell reactions, Applications of EMF measurements: Equilibrium constant, Thermodynamic parameters, Potentiometric titrations; Basic principles of ion- selective membrane electrodes, Batteries, Bioelectrochemistry.
-
- **Statistical Thermodynamics**
  The Canonical Ensemble, Canonical Partition Function for a System of Noninteracting Particles, Canonical Partition Function of a Pure Ideal Gas, The Boltzmann Distribution Law for Non-interacting Molecules, Statistical Thermodynamics of Ideal Monatomic and Diatomic Gases, Statistical Thermodynamics of Ideal Polyatomic Gases, Equilibrium Constants, Entropy and the Third Law of Thermodynamics.

Course Outcomes:

- Understanding the laws of Thermodynamics and phase equilibrium of multicomponent systems
- Understanding the thermodynamics of surfaces and different adsorption isotherms of gases on solids
- Key concepts for Electrochemistry and its applications.
- Concepts of Statistical Thermodynamics.

References:

1. Physical Chemistry, I. Levine, Tata McGraw Hill, 5th Edn., 2007.
2. Physical Chemistry of Surfaces, A. W. Adamson and A. P. Gast, John Wiley and Sons, Inc., 1997.
3. Modern Electrochemistry, J. O. M. Bockris and A. K. N. Reddy, Springer, 2006.
4. Physical Chemistry, R. S. Berry, S. A. Rice and J. Ross, Oxford Univ. Press, 2nd Edn., 2000.
5. Physical Chemistry, P. W. Atkins and J. de Paula, W. H Freeman and Company, 9th Edn., 2010.

C301: Physical Organic Chemistry (CHE-301-C) (45 L+15T)

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

Course Details:

- **Stereo electronic 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. [10]

- **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 Woodward–Hoffmann Rules and Molecular Orbitals and their 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.

C303: Physical Methods in Chemistry I (CHE-303-C) (45 L+15T)

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

Course Details:

- **General Introduction to Spectroscopy**
  Electromagnetic radiation and its interaction with atoms and molecules. Holistic view of spectroscopy.

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

- **Mass Spectrometry**
  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.

Course Outcomes:

- Understand the basics of absorption and fluorescence spectroscopy.
- Theoretical prediction of absorption maximum of some organic molecules.
- Identifying and distinguishing various types 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 (Sensing applications).

References:

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.
6. Principles of Molecular Photochemistry: An Introduction, P. Walsh, N. J. Turro,
7. V. Ramamurthy, J. C. Scaiano, University Science Books, 2008.
8. Principles of Fluorescence Spectroscopy. Joseph R. Lakowicz, 3rd Edn., Springer, 2006.
9. Interpretation of Mass Spectra, F. W. McLafferty, 1980.
10. Spectrometric Identification of Organic Compounds, R. M. Silverstein, G. C. Bassler and T. C. Morrill, John Wiley, New York

C305: Molecular Quantum Mechanics (CHE-305-C) (45 L+15T)

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 diatomics, Valence-Bond Method.

- Hückel Molecular Orbital theory and Introduction to Hartree method. [4]

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

C302: Coordination Chemistry (CHE-302-C) (45 L+15T)

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. [10]

- **Magnetism**
  Introduction to Magnetism. Origin of diamagnetism. Paramagnetism: 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 Antiferromagnetic; 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**
  Substitution Ligand design and applications.

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 chemistry

References:

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

C304: Molecular Spectroscopy and Group Theory (CHE-304-C) (45 L+15T)

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.

- **Polyatomic 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.

References:

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.

C306: Physical Methods in Chemistry II (CHE-306-C) (45 L+15T)

Coordinators: Prof. A. Srinivasan
srini@niser.ac.in

Course Details:

- **Nuclear Magnetic Resonance Spectroscopy**
  Basic principles, Chemical shifts, Spin-spin interactions; Application of 1H and 13C NMR spectroscopy including NOE, COSY, NOESY, and other 2D techniques in the structure determination of bioorganic compounds; Application in conformational analysis. Multinuclear (31P, 19F, 29Si) NMR of various inorganic and organo- metallic compounds. Instrumental aspects; NMR of paramagnetic sample: Contact shifts and pseudo contact shifts, Shift reagents; Pulsed NMR: Modern multiple- pulsed experiments including 2D NMR.

- **Electron Spin Resonance Spectroscopy (ESR)**
  A brief review of theory; Analysis of ESR spectra of systems in liquid phase; Radicals containing single set; Multiple sets of protons; Triplet ground states: Transition metal ions; Fe, Cu, Mo, Cr, Mn, VO2+ containing systems: g values; Symmetry; The practical interpretation of ESR spectra in solid state and solution states; Multiple electron systems; Triplet ground state, Zerofield splitting, Kramers degeneracy, Spectral line-shapes when D « hν, D ~hν and D » hν. EPR of photoexcited triplet states.

- **Double resonance Techniques (ENDOR)**
  ENDOR in liquid solution, ENDOR in powders and non-oriented solids; ENDOR spectra of free-radicals coupled to multiple sets of nuclei with spin; ENDOR of paramagnetic metals and complexes; Biological Applications: Substrate free radical; Flavins and metal free flavin proteins; Photosynthesis; Heme proteins; Iron–Sulfur proteins; Spin labels.

- **Mossbauer Spectroscopy**
  Basic physical concepts; Spectral line shape; Isomer shift; Quadrupole splitting, Magnetic hyperfine interaction; Interpretation of Mossbauer parameters of 57Fe, 99Ru, 101Ru, 195Pt, 193Ir, and 110Sn; Some special applications: Solid state reactions; Thermal decomposition, Ligand exchange, Electron transfer, Isomerism, Surface studies and biological applications.

Course Outcomes:

- To learn instrument techniques such as NMR and EPR.
- To interpret the data obtained from these techniques.
- To understand various aspects involved in NMR, EPR, ENDOR and Mossbauer.
- To find out the radical nature of the materials.

References:

1. NMR Spectroscopy: Basic principles, Concepts and Applications in Chemistry,
2. H. Gunther, 2nd Edn. John Wiley & Sons, 1995.
3. Spectrometric Identification of Organic Compounds, R. M. Silverstein, G. C. Bassler and T. C. Morrill, John Wiley, New York, 5th Edn., 1991.
4. Basic 1H and 13C NMR Spectroscopy, M. Balci, Elsevier Science, 2005.
5. Electron paramagnetic Resonance: Elementary Theory and practical applications, J. A. Weil, J. R. Bolton and J. E. Wertz, Wiley Interscience, New York, 1994.
6. Physical Methods in Chemistry, R. S. Drago, 2nd Edn., Saunders, 1992.
7. Mossbauer Spectroscopy: An Introduction for Inorganic Chemists and Geochemists, Mcgraw Hill, UK, 1973.
8. Mossbauer Spectroscopy, N. N. Greenwood and T. C. Gibb, Chapman & Hall, 1971.
9. Electron Spin Resonance: Elementary Theory and Practical Applications, J. E. Wertz and J. R. Bolton, Mcgraw Hill, 1984.

C401: Chemistry of Heterocycles and Natural Products (CHE-401-C) (45 +15T)

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.

References:

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.

C403: Chemical Rate Processes (CHE-403-C) (45 L+15T)

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

Course Details:

- **Kinetic Measurements**
  General features of fast reactions; Study of fast reactions by flow techniques, Relaxation methods (T-Jump, P-Jump, ultrasonic, pulse radiolysis, NMR); Flash photolysis; Salt and solvent effects on reactions in solutions.

- **Chain Reactions**
  Features of chain reactions; Thermal and photochemical reactions (hydrogen–bromine reaction, decomposition of aldehydes and ketones).

- **Kinetics of oscillatory reactions**
  Introduction to oscillatory reactions; Belousov- Zhabotinsky and Field-Koros-Noyes models.

- **Rate Theory**
  Concept of potential energy surfaces, Transition state theory including its statistical mechanical treatment, Phenomenological theories of unimolecular reactions (Lindemann, Hinshelwood), Statistical mechanical theories of unimolecular reactions (RRKM).

- **Chemical Dynamics**
  Collision theory and Reaction Dynamics, Reaction Cross section and rate constant, Brief idea of Molecular Beam Scattering, Dynamics in condensed phase.

- **Femtochemistry**
  Concepts and perspectives; Applications to studies of dynamics and control of chemical reactions. [6]

Course Outcomes:

- Students can learn varieties of chemical reactions and the time scale of those reactions.
- Describes different spectroscopy and analytical techniques to study chemical kinetics.
- Introduces enzyme kinetics.
- It is a useful course for chemistry and biology students to learn about chemical and biological reactions.

References:

1. Physical Chemistry, I. Levine, Tata Mcgraw Hill, 5th Edn., 2007.
2. Physical Chemistry: A Molecular approach, D. a. McQuarrie and J. D. Simon, University Science Books, 1997.
3. Chemical Kinetics and Dynamics, J. I. Steinfeld, J. S. Francisco and W. L. Hase, Prentice Hall, 1999.
4. Chemical Dynamics in Condensed Phases: Relaxation, Transfer and Reactions in Condensed Molecular Systems, A. Nitzan, Oxford Univ. Press, 2006.

References:

1. Basic Chemical Kinetics, H. Eyring, S. H. Lin and S. M. Lin, John Wiley & Sons, New York, 1980.
2. The World of Physical Chemistry, K. J. Laidler, Oxford University press, 1993

ELECTIVE COURSES

C351: Photochemistry (CHE-351-C) (45 L+15T)

Coordinators: Dr S. Peruncheralathan
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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.

- **Applied Photochemistry**
  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.

References:

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,
5. V. Ramamurthy, J. C. Scaiano, University Science Books, 2008.
6. Organic photochemistry, J. M. Coxon and B. Halton, Cambridge University press, 1974.
7. Molecular Reactions and Photochemistry, C. H. Depuy and O. L. Chapman, Prentice Hall of India.
8. Photochemistry and Pericyclic Reactions, J. Singh and J. Singh, New Age International Publishers, 2003.
9. Pericyclic Reactions, I. Fleming, Oxford Science Publications 1998.

C352: Pharmaceutical Chemistry (CHE-352-C) (45 L+15T)

Coordinators: Dr S. Peruncheralathan
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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 the AMDE principle of drugs (absorption, distribution, metabolism, and excretion).
- To understand drug discovery processes.

References:

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

C353: Classics in Molecules (CHE-353-C) (45 L+15T)

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. [7]
- 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 the discovery of organic molecules and their impact on the world, such as Urea, Glucose, & Penicillin.
- To understand the introductory organic chemistry for learning chemical biology.
- To learn about the small organic molecules that interact with molecular targets.
- To find the nature of drugs and their function in biological changes.

References:

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.

C551: Molecular Modeling (CHE-551-C) (45 L+15T)

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**
  Hartree–Fock-Self-Consistent-Field theory, Post- Hartree–Fock (Electron correlation) methods, Density functional theory, Semi- empirical methods.

- **Chemical Dynamics**
  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. [10]

Course Outcomes:

- Construct 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

References:

1. C. J. Cramer, Essentials of Computational Chemistry, Wiley, 2004.
2. I. N. Levine, Quantum Chemistry, Prentice-Hall of India, 2006.
3. P. W. Atkins, Molecular Quantum Mechanics, Oxford, 2008.
4. P. Allen and D. J. Tildesley, Computer Simulation of Liquids, Oxford, 1987.
5. R. Leach, Molecular Modelling, Prentice Hall, 2001.
6. F. Jensen, Introduction to Computational Chemistry, John Wiley & Sons, 2007.

C552: Solid State Chemistry (CHE-552-C) (45 L+15T)

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. [8]

- **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:**
  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

References:

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.

C554: Crystallography (CHE-554-C) (45 L+15T)

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. [4]

- 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. [14]

- 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. [14]

- 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. [10]

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

References:

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

C555: Principles of Drug Action (CHE-555-C) (45 L+15T)

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 trials
- To find the modern drug discovery and development processes including the identification of molecular targets, High-throughput screening (HTS)

References:

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.

C556: Advanced Bio-inorganic Chemistry (CHE-556-C) (45 L+15T)

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.

- **Iron–Sulfur Proteins**
  Types, function and mechanisms, Rubredoxin, Ferredoxins, Aconitase.

- **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).

- **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). [4]

- **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 for particular functions.
- 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.

References:

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.

C557: Nuclear Magnetic Resonance (CHE-557-C) (45 L+15T)

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.

References:

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.

C558: Advanced Functional Materials (CHE-558-C) (45 L+15T)

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 interdisciplinary sciences
- Use of polymer materials and nanocomposites in chemistry and day-to-day life

References:

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.

C559: Supramolecular Chemistry (CHE-559-C) (45 L+15T)

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. [20]

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

References:

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,
4. D. D. Macnicol, F. Vogtle, Volumes 2 and 3, Elsevier Science, Oxford, 1996.
5. Supramolecular Chemistry of Anions, Edn. A. Bianchi, K. Bowman-James, E. Garcia- Espana, John Wiley and Sons, New York, 1997.
6. Supramolecular Chemistry, P. D. Beer, P. A. Gale and D. K. Smith, Oxford University Press, 1999.
7. A Practical Guide to Supramolecular Chemistry, Peter J. Cragg, John Wiley & Sons Ltd, England, 2005.

C560: Chemistry of Nanomaterials (CHE-560-C) (45 L+15T)

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.

- **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
- Use of nanomaterials in energy and biological applications

References:

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.

C561: Advanced Bio-organic Chemistry (CHE-561-C) (45 L+15T)

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 Biomacromolecules, and Enzymology
- Synthesis and application of DNA, RNA and related analogues
- Understanding of biosynthesis of natural products
- Understanding the role biomacromolecules in therapy

Recommended Books:

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
4. A. Copeland, Publisher: Wiley- interscience; 2005.

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

C562: Polymer Chemistry (CHE-562-C) (45 L+15T)

Coordinators: Prof. V. Krishnan
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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. [10]

- 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.

- 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 biodegradable polymers

References:

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.

C563: Molecular Reaction Dynamics (CHE-563-C) (45 L+15T)

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 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

References:

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.

C564: Theory of Molecular Spectroscopy (CHE-564-C) (45 L+15T)

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

References:

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.

C565: Advanced Organic Chemistry (CHE-565-C) (45 L+15T)

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. [42]

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

References:

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. F. A. Carey, R. J. Sundberg, “Advanced Organic Chemistry Parts A & B: Structure and Mechanisms” 5th Edn., Springer, 2007.
4. B. Smith, J. March “Advanced Organic Chemistry” 6th Edn., Wiley-VCH, 2007.
5. E. J. Corey, X.-M. Cheng, “The Logic of Chemical Synthesis” Wiley- interscience, 1995.
6. T. Hudlicky, J. W. Reed, “The Way of Synthesis: Evolution of Design and Methods for Natural Products” Wiley-VCH, 2007.
7. P. Wyatt, S. Warren, “Organic Synthesis: Strategy and Control” Wiley, 2007.
8. Christmann, S, Brase Eds “Asymmetric Synthesis- The Essentials” 2nd Edn., Wiley-VCH, 2008.
9. K. C. Nicolaou, R. Hanko, W. Hartwig Eds. ”Handbook of Combinatorial Chemistry”, VCH-Wiley, Weinheim, 2002.
10. R. Bruckner, “Organic Mechanisms: Reactions,Stereochemistry and Synthesis” Springer, 2010.

C566: Advanced Organic Chemistry (CHE-566-C) (45 L+15T)

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

References:

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.

C567: Advanced Main Group Chemistry (CHE-567-C) (45 L+15T)

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

Course Details:

- **Direct Bonds Between Metal Atoms**
  Mg and Ca compounds with metal- metal bonds (b) 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

References:

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.

C568: Advanced Fluorescence Spectroscopy (CHE-568-C) (45 L+15T)

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

References:

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.

C569: Bio macromolecules (CHE-569-C) (45 L+15T)

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

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). [9]

- 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

References:

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.

C570: Advanced Heterocyclic Chemistry (CHE-570-C)) (45 L+15T)

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

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
- Recent methods of C-H functionalization/activations of heterocyclic derivatives.

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

References:

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.

C571: Statistical Mechanics (CHE-571-C)) (45 L+15T)

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

References:

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.

C572: Frontiers in Organic Synthesis (CHE-572-C) (60 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

References:

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

C573: Chemical Binding (CHE-573-C) (60 Hours)

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

Course Details:

- **Introduction**
  Review of basic principles of quantum mechanics, Atomic structure, Variation and perturbation methods.

- **Electronic structure of diatomic molecules**
  Born–Oppenheimer approximation, H_2^+ ion, Molecular orbitals of ground state and excited states of H_2^+ (LCAO-MO), Homo and heteronuclear diatomic molecules, Electronic term symbols, Valence Bond Theory of diatomic molecules, Comparison of VB and MO theories. Term symbols for diatomic molecules.

- **Self-consistent Field methods**
  Hartree–Fock theory of atoms and molecules, Post-Hartree–Fock theories, Configuration interaction wave functions.

- **Electronic structure of polyatomic molecules**
  SCF-MO treatment of closed shell systems and applications to molecules (H_2O, NH_3, CH_4); Potential energy surface and equilibrium geometry, Molecular vibrational frequencies. Brief introduction to density functional theory.

- Virial theorem and chemical bonding. The Hellman–Feynman theorem.

- Semi-empirical and molecular mechanics treatment of molecules, Huckel molecular orbital theory for conjugated organic molecules and its applications to Ethylene, Butadiene, Benzene; Delocalization energy and stability.

Course Outcomes:

- Understand the quantum mechanics of molecules
- Construct molecular orbitals for polyatomic molecules
- Apply symmetry and molecular orbital theory to derive molecular terms
- Understand the Hartree-Fock (HF) theory, DFT, and semi-empirical methods

References:

1. Modern Quantum Chemistry: Introduction to Advanced Electronic Structure, A. Szabo and N. S. Ostlund, Dover, 1996.
2. Molecular Quantum Mechanics, P. W. Atkins and R. S. Friedman, Oxford University Press, 3rd Edn., 1997.
3. Quantum Chemistry, I. N. Levine, 5th Edn., Pearson Education, 2000.

LABORATORY EXPERIMENTS

CHE141: Chemistry Laboratory-I (CHE-141-C) (60 Hours)

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

Course Details:

- Determination of the heat of solution of oxalic acid by measuring its solubility at various temperatures.
- Determination of the rate constant for the acid-catalyzed hydrolysis of methyl acetate.
- Study of the kinetics of the iodide-hydrogen peroxide clock reaction.
- Determination of the concentration of an unknown solution using turbidimetry.
- pH-metric titration of a weak acid against a strong base.
- Verification of Beer-Lambert's law.
- Spectrophotometric analysis of caffeine and/or benzoic acid in soft drinks.
- Synthesis of hexamine nickel (II) chloride.
- Preparation of potash alum.
- Synthesis of aspirin.
- Synthesis of methyl orange.
- Cyanotype blueprinting.
- Estimation of calcium in milk powder using EDTA complexometry.
- Extraction of caffeine from tea leaves.
- Element detection and characterization of organic compounds.

Course Outcomes:

- Demonstrate analytical skills in measuring, interpreting, and analyzing experimental data.
- Develop laboratory skills in synthesis, titration, and extraction techniques.
- Apply problem-solving abilities to chemical kinetics and thermodynamic studies.
- Gain proficiency in using modern analytical instruments like spectrophotometers and pH meter.

References:

1. The Systematic Identification of Organic Compounds, R. L. Shriner, C. K. F. Hermann, T. C. Morrill, D.
2. Curtin and R. C. Fuson, John Wiley, 8th Edn., 2004.
3. Practical Organic Chemistry, A. I. Vogel, ELBS, 2002.
4. Laboratory Manual in Organic Chemistry, R. K. Bansal, Wiley Eastern, 1980.
5. Comprehensive Practical Organic Chemistry: Qualitative analysis, V. K. Ahluwalia and S. Dhingra, Universities Press (India) Ltd, 2000.
6. A Collection of General Chemistry Experiments, A. J. Elias, Universities Press, 2007.
7. Experimental Physical Chemistry, R. C. Das and B. Behera, Tata Mcgraw Hill, 1983.
8. Practical Physical Chemistry, A. Findlay and J. A. Kitchener, 8th Edn., Longmans, 1967.

CHE241: Chemistry Laboratory-I (CHE-241-C) (120 Hours)

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

Course Details:

- Inorganic (Carbon-Free) Chelate rings: A Dithioimidodiphosphinato ligand and some of its metal complexes.
- Synthesis of [Ti(urea)6]I3: An air-stable d1 Complex.
- Synthesis, Electrochemistry and Luminescence of [Ru(bpy)3]2+
- Synthesis and Electrochemistry of Ferrocene and its Derivatives.
- Standardisation of sodium thiosulphate solution and volumetric estimation of Cu (II) iodometrically.
- Volumetric estimation of Zn (II), Ca (II) and Mg (II) by EDTA titration, using Eriochrome black-T indicator.
- Gravimetric estimation of nickel (II), using dimethylglyoxime.
- Estimation of: (a) total manganese content in manganese ore (pyrolusite); (b) total iron content in Fe2O3 (haematite).
- Study of the composition of ferric-sulfosalicylic acid complex by Job's method of continuous variation, and to determine the stability of the complex, spectrophotometrically.
- Determination of the composition of a binary mixture (potassium Dichromate and potassium permanganate) using spectrophotometry.
- Synthesis of 3,5-dimethyl pyrazole.
- Solid phase synthesis of trans-bis glycinato copper(II) complex.
- Synthesis of Fe(salen)Cl complexes; B) Elucidation of Redox behavior of Fe(III) and C) Elucidation of magnetic properties.
- Synthesis of meso tetratolyl 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 $[Co(NH_3)_5Cl]Cl_2$.
- Friedel-Craft acylation of ferrocene.

Course Outcomes:

- Concepts used in inorganic experiments
- Laboratory procedures to perform inorganic experiments
- 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 the ion exchange column, which is used in the pharmaceutical Industry.
- Able to clearly communicate the results of scientific work in oral, written and electronic formats to both scientists and the public at large.

References:

1. Vogels Textbook of Qualitative Chemical Analysis, G. H. Jeffery, J. Bassett, J. Mendham and R. C. Denny, 5th Edn., ELBS, 1991.
2. Handbook of Preparative Inorganic Chemistry, Vol. i & ii (edited by G. Brauer), Academic Press, 1963.
3. Experimental Electrochemistry for Chemists, D. T. Sawyer and J. L. Roberts, Jr., John Wiley & Sons, New York, 1974.
4. Vogels Textbook of Quantitative Chemical Analysis, G. H. Jeffery, J. Bessett, J. Medham and R. C. Denny, 5th Edn., ELBS, 1999.

CHE242: Organic Chemistry Laboratory (CHE-242-C) (120 Practical Hours)

Coordinators: Dr. S. Peruncheralathan
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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:
  - Diels-alder reaction of anthracene and Maleic anhydride
  - Synthesis of Cinnamic acid from Benzaldehyde (perkin reaction)
  - Synthesis of Triphenyl Carbinol (Grignard Reaction)
  - Synthesis of 2-hydroxy-5-methyl benzophenone (Fries rearrangement)
  - Synthesis of Benzilic acid from Benzil (Benzil-Benzilic acid rearrangement)
  - 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 Beckmann rearrangement.
- Synthesis of Bisnaphthol.
- Synthesis of 3,4-dihydropyrimidin-2(1H)-ones using Biginelli reaction, a multi- component chemical reaction.

Course Outcomes:

- Develop analytical skills for quantifying and characterizing chemical and biological compounds using chromatography, spectroscopic, and biochemical techniques.
- Master synthetic organic chemistry techniques, including classical name reactions, multi-step synthesis, and rearrangement reactions.
- Gain proficiency in advanced laboratory techniques, such as protection- deprotection strategies, esterification, and solvent preparation.
- Apply modern instrumental methods (IR, NMR, UV-Vis) for the identification and characterization of organic compounds.
- Demonstrate problem-solving and critical-thinking skills in designing and executing multi-step syntheses and chemical transformations.
- Explore heterocyclic and biologically active compound synthesis, including coumarins, indoles, and caprolactam.
- Conduct multi-component and industrially relevant reactions for efficient synthesis of complex molecules.

References:

1. Intermediates for Organic Synthesis, V. K. Ahluwalia, P. Bhagat, R. Aggarwal,
2. R. Chandra, I. K. International, New Delhi, 2005.
3. Practical Heterocyclic Chemistry, A. O. Fitton and R. K. Smalley, Academic Press, London, 1968.
4. Vogel's Textbook of Quantitative Chemical Analysis, G. H. Jeffery, J. Bassett,
5. J. Mendham, and R. C. Denny, 5th Edition, ELBS, 1991.
6. Spectrometric Identification of Organic Compounds, R. M. Silverstein, G. C. Bassler, and T. C. Morrill, 6th Edition, Wiley, 1998.
7. A Collection of Interesting General Chemistry Experiments Anil J. Elias, Universities Press, 2007.
8. Laboratory Manual of Organic Chemistry, B. B. Dey and M. V. Sitaraman, Allied Publishers, 1992.
9. Laboratory Manual of Organic Chemistry, R. K. Bansal, New Age International Publishers, 2006.

CHE341: Physical Chemistry Laboratory (CHE-341-C) (120 Practical Hours))

Coordinators: Prof. Himansu S. Biswal
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Course Details:

- Study of the pH dependence of UV-Visible spectrum of 4-nitrophenol/methyl orange and determination of its pK by spectrophotometric method.
- Study of the kinetics of inversion of cane sugar, catalyzed by acid, polarimetrically.
- Study of the dimerization of benzoic acid by partition method.
- Adsorption of acetic acid on activated charcoal, and verification of Freundlich / Langmuir adsorption isotherm.
- Verification of Beer–Lambert's Law and determination of the dissociation constant (pKa) of methyl red, spectrophotometrically.
- Study of the phases diagram of a two-component system (diphenylaminebenzophenone) with congruent melting point.
- Determination of the isotherm for a three-component system (diphenylamine- acetic acid-water).
- Determination of glass transition temperature of hydrated calcium nitrate, conductometrically.
- Estimation of halides in a mixture of halides by potentiometric titrations.
- Study of the Solvent Effects on the fluorescence of fluorescein and other fluorescent molecules.
- Study of the kinetics of the iodide - hydrogen peroxide clock reaction.
- Study of the photochromic and kinetic behaviour of a nitrospiropyran derivative.
- Determination of the bond lengths of diatomic and triatomic molecules and Functional group determination of small molecules using the FT-IR spectrometer.
- Quantum Yield Calculation for anthracene.
- Fluorescence Quenching by KI.
- Solvatochromic study of a Donor acceptor system.
- Static and Dynamic Fluorescence quenching and verification of the Stern- Volmer relationship.

Course Outcomes:

- Develop analytical skills in spectrophotometry for determining physical constants like pKa and studying pH-dependent properties.
- Understand reaction kinetics and mechanisms through experimental studies of chemical processes.
- Investigate thermodynamic and equilibrium properties using methods such as partitioning, phase diagrams, and adsorption studies.
- Gain proficiency in advanced instrumental techniques like FT-IR, fluorescence spectroscopy, and potentiometric titrations for molecular analysis.
- Explore molecular interactions and properties through fluorescence studies, including quenching and solvatochromic effects.
- Apply photochemistry and quantum mechanics concepts to calculate quantum yields and analyze photochromic behavior.
- Study multi-component systems and isothermal behavior using experimental techniques.

References:

1. Experimental Physical Chemistry, R. C. Das and B. Behera, Tata McGraw-Hill, 1983.
2. A Collection of Interesting General Chemistry Experiments, A. J. Elias, Universities Press, 2007.
3. Experimental Physical Chemistry, V. D. Athawale and P. Mathur, New Age International Publishers, 2001.
4. Experimental Physical Chemistry: A Laboratory Textbook, A. M. Halpern, Prentice Hall, 2nd Edition, 1997.
5. Practical Physical Chemistry, A. Findlay and J. A. Kitchener, 8th Edition, Longmans, 1967.

CHE342: Computational Chemistry Laboratory (CHE-342-C) (120 Practical Hours)

Coordinators: Prof. U. Lourderaj
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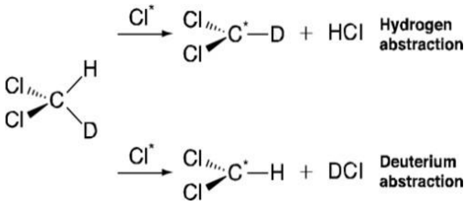
Course Details:

- 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 of protonated water clusters (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

References:

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.