Integrated M. Sc-Ph. D Programme

at

School of Chemical Sciences

National Institute of Science Education and Research (NISER), Bhubaneswar

Contents

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1. Introduction

Integrated M. Sc-Ph. D programme at the School of Chemical Sciences (SCS), NISER, Bhubaneswar is a newly added programme and is expected to commence from the academic year 2022.

2. Admission

The minimum qualification for admission to the programme is Bachelor's degree in **Chemistry** or an equivalent degree from a university recognized by UGC.

Prospective candidates will be shortlisted based on their performance in national level entrance exams like JAM. The shortlisted candidates will be interviewed at NISER, Bhubaneswar.

3. The Academic Programme

- The Integrated M. Sc -Ph. D programme at NISER shall consist of: (i) Course work involving classroom courses as well as a research project leading to the award of the M. Sc degree (3 years), and (ii) Research work leading to a Ph. D thesis and the award of Ph. D degree.
- Duration of Integrated M.Sc.-Ph. D. programme is 6 years (or 7 years for dual degree MSc and Ph.D).
- The course work for the Integrated M. Sc-Ph. D programme will be based on courses that have been approved by the Academic Council of NISER. The details are given in section 4. The duration of the course work shall be equivalent to three academic years which includes two class room teaching and one year project work. Approximately one third of the course credits are to be earned through a Master's project leading to a Master's thesis.
- The evaluation of the students will be based on continuous assessment (quizzes/homework etc.) and examinations. The Master's project will be evaluated in each semester by the school and the thesis will have to be defended in an open thesis defense. The students who have a CGPA of 7.0 or more at the end of two years and successfully defended their Master's thesis at the end of the third year of the programme shall be eligible for the award of the Master's degree.
- Students who are unsuccessful in earning a CGPA of 7.0 after the first two years shall be considered ineligible for the M. Sc. degree.
- For the continuation of studies towards a Ph. D. degree, the students will be required to take a General Comprehensive Examination (GCE) based on the courses attended during the M. Sc course work. This exam. can be taken once students have completed all the course requirements for the M.Sc. degree other than the research project. On satisfactory performance in the GCE and the successful completion of the M Sc. course work, the PGCS can recommend the student to register for a Ph.D. after informing the PGCI.
- A student will at most be allowed two attempts to pass the General Comprehensive Examination (GCE). A student failing to pass the GCE twice will be deemed ineligible for registering for Ph.D. degree.
- The programme will be conducted according to the rules and regulations of the HomiBhaba National Institute (HBNI), of which NISER is a constituent institute. On admission to the Integrated M. Sc-Ph. D programme, the students will be registered with HBNI. They will receive an M.Sc degree after three academic years, and on passing the GCE, they can continue

research towards a Ph. D degree. The rules of the Homi Bhabha National Institute (HBNI) regarding the award of the Ph. D degree will apply during this period.

4. **Fellowship**

The students of this programme will receive a monthly stipend of Rs. 21,000/- for the first year and Rs. 31,000/- in the next two years and Rs. 35,000/- upto 7th year. A contingency grant, housing, and medical facilities will be provided as per DAE rules.

5. **Course structure**

The course work in the Integrated M. Sc-Ph. D program for the award of an M. Sc degree will span three academic years. The total number of course credits required for the award of the M. Sc degree at the end of three years is proposed to be 228. The classroom teaching is proposed to be completed in two years. The workload is proposed to be distributed across the three years. At SCS, NISER, most theory courses are 8-credit courses (3 hours of lectures and 1 hour tutorial per week). For a laboratory course, 3-credits are usually equivalent to one laboratory session lasting 3 hours. NISER currently has two different sets of courses for its Integrated M. Sc programme and the Ph.D programme. It is proposed that the courses to be taken by the incoming Integrated M. Sc-Ph. D students be a mix of courses from the Ph. D programme and those taken by advanced undergraduates of the Integrated M. Sc programme. In addition, new courses are also proposed. The semester-wise distribution of courses for meeting the course requirements are as follows. The syllabi are given in the Appendices.

4.1 First Year

Semester	Course No.	Credits	Course Name
Semester-I	C701	8	Physical Organic Chemistry
	C702	8	Molecular Quantum Mechanics
	C703	8	Chemistry of Main Group (s and p-block) Elements
	C741	6	Organic Chemistry Laboratory-I (6hr/week)
	C742	6	Inorganic Chemistry Laboratory-I (6hr/week)
Semester-II	C704	8	Molecular Spectroscopy and Group theory
	C705	8	Coordination Chemistry
	C706	8	Advanced Organic Chemistry
	C743	6	Organic Chemistry Laboratory-II (6hr/week)

	C744	6	Physical Chemistry Laboratory, 6hr/week
4.2 Second Year			
Semester-III	C801	8	Heterocyclic and Natural Product Chemistry
	C802	8	Organometallic Chemistry
	C803	8	Applied Spectroscopy-I
	****	8	Elective - I
	C841	6	Inorganic Chemistry Laboratory-II, (6hr/week)
Semester-IV	C804	8	Applied Spectroscopy-II
	C842	6	Computational Chemistry Lab, 6hr/week
	****	8	Elective II
	****	8	Elective III
	C843	8	Research Laboratory, 8hr/week contact hours

4.3 Third Year

The third year of course work will entirely consist of research work for the Master's project. The project consists of 40 credits and is started in the 5th semester as shown above. After the completion of the project, the student can continue research work towards a Ph. D degree if the performance in the oral comprehensive examination is deemed satisfactory. Thereafter PhD. Guide will be assigned.

Semester	Course Code	Credit	Courses, Code, Credit
Semester-V	C901	40	Specific-Research Works for M. Sc.
	****	4#	Research Methodology (Only for PhD)
Semester-VI	C902	40	Specific-Research Works for M. Sc.
	****	2#	Research and publication ethics (Only for PhD)

#: Confirmation is required from Deans' Offices

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6. **Appendix A**

All theory courses (Core/Elective courses) are 8-credit courses (3 hours of lectures and 1 hour tutorial per week, 15 weeks (including exams).

C701: Physical Organic Chemistry

Course Outcomes:

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

1. *Stereoelectronic* Effects: Anomeric & related effects; Acetals, Esters, Amides and related functions; Reactions at sp3, sp2, and sp Carbons; Examples in synthesis and biological processes; Felkinahn Model, Houk Model, Cieplak Model, EFOE Model, and Cation-complexation model as applied to π-Facial Selectivity; Baldwin's Rule.
2. *Pericyclic Reactions*: The nature of pericyclic Reactions; The Woodward-Hoffmann Rules and Frontier 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 Reaction.
3. *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.
4. *Radical Reactions*: Generation and Characterization of Free Radicals; Nucleophilic and Electrophilic Radicals; Substitution Reaction; Addition Reactions; Radical Coupling; Barton Reaction.

Recommended Books:

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.

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C702: Molecular Quantum Mechanics

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

Course Details:

1. *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.
2. *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.
3. *Approximation Methods*: Variational and perturbation methods
4. Atomic Structure: Electron Spin, Helium Atom and the Spin–Statistics Theorem, Total Orbital and Spin Angular Momenta, Many-Electron Atoms, Atomic Terms.
5. *Molecular Electronic Structure*: Born–Oppenheimer Approximation, Hydrogen Molecule Ion, Simple Molecular Orbital Method for Diatomic Molecules, Molecular Terms for diatomic, Valence-Bond Method.
6. Hückel Molecular Orbital theory and Introduction to Hartree method.

Recommended Books:

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

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C703: Chemistry of Main Group (s and p-block) Elements

***Course Outcomes*:**

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

1. Chemistry of alkali and alkaline earth elements: Structure and bonding in alkali and alkaline earth metal Complexes-Alkali metal chemistry with carbon based ligands and Group 14 and 15 alkali metal bonded complexes. Low oxidation state with M-M bonded alkaline earth metal complexes; Synthesis and reactivity studies.
2. Chemistry of Boron, Aluminum and Silicon: Boranes, Carboranes and heterocarboranes, Multiple bonded main group compounds containing B-B double and triple bonds, Al-Al double bond and Si-Si double and triple bonds: Synthesis and reactivity studies.
3. Main group metal compounds in Homogenous Catalysis: Group 2 metal complexes in catalytic reactions such as hydroboration, hydrosilylation, hydroamination, dehydrocoupling, hydrogenation and hydrophosphination.
4. Group 13 and 14 (B, Al, Si and Ge) based molecular compounds in homogenous catalysis.

Recommended Books

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

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C704: Molecular Spectroscopy and Group Theory

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.

Course Details:

1. Group Theory: Symmetry elements, Symmetry operations, Point groups, Symmetry representations; Definition of a group and basic theorems, Molecular symmetry groups and classes, Matrix representation of symmetry operations, Reducible and Irreducible representations, Great Orthogonality Theorem; and Character Tables, direct product of irreducible representations.
   Application to Quantum Chemistry: Symmetry properties of wave functions, Orbitals as basis for irreducible representations, Projection Operator, Symmetry adapted linear combinations, Assignment of symmetry representations of d-orbitals for specific geometries.
   Applications of symmetry to Molecular Orbital diagrams of simple molecules (examples: H_2O, BeH_2, $BF_3(\sigma + \pi)$); Huckel molecular orbital theory for conjugated molecules.

2. Introduction to Spectroscopy: Interaction of light with matter, Time-dependent perturbation theory, Transition moment integral and transition probabilities, Selection Rules, Einstein's coefficients, Oscillator strength, Broadening and width of spectral lines.
3. Diatomic Molecules: (a) Electronic Spectra: Born-Oppenheimer approximation, Potential energy curves of diatomic molecules, Frank-Condon principle, Electronic transitions in homonuclear and heteronuclear diatomics.
   (b). Microwave and Infrared Spectroscopy: Simple harmonic oscillator and Rigid Rotor Model, Rotational spectra of diatomic molecules, Stark effect, Vibrational spectra of diatomic molecules, An harmonic correction, Selection rules, Fundamental and Overtone bands, Isotope effects, Vibrational Rotational coupling, etc.
4. Polyatomic Molecules:
   (a). Electronic Spectra: Electronic structure, Electronic spectra of polyatomic molecules - linear conjugated molecules, Aromatic molecules, Transition metal compounds, Fluorescence, Phosphorescence, Internal conversion and Charge transfer.
   (b). 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. Prediction of IR and Raman active modes using group theory.

Recommended Books:

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.
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.

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C705: Coordination Chemistry

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

Course Details:

1. *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.
2. *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 Antiferromagnetism; Bulk magnetic properties and ferromagnetism; Molecule-based magnetic materials: Organic magnets and single molecule magnets.
3. *Mechanisms of reactions of transition metal complexe*s: Substitution (Kinetic effects: labile vs inert) and electron- transfer reactions (Outer-sphere, Self- exchange; Inner-sphere).
4. *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: Hemeerythrin, Ribonucleotide reductase, Methanol monooxygenase (a) Iron-Sulfur proteins: Ruberodoxin, Ferredoxin; (b) DNA / RNA: Ribozymes.
5. *Transition metal based supramolecular structures***:** Ligand design and applications.

Recommended Books:

1. Advanced inorganic Chemistry, F. A. Cotton, C. A. Murillo, and M. Bochmann, Wiley Inter science, 2001.
2. Inorganic Chemistry, D. F. Shriver and P. W. Atkins, Oxford University Press, 1999.
3. Supramolecular Chemistry: Concepts and Perspectives, J. M. Lehn, VCH, 1995.
4. Principles of Bioinorganic Chemistry, S. J. Lippard and J. M. Berg, Panima Publications, New Delhi,1997.
5. Bioinorganic Chemistry; Inorganic Elements in the Chemistry of Life. Kaim, B. Schwederski Wiley, 1994.
6. Biological Inorganic Chemistry: Structure and Reactivity Harry B. gray, E. I. Stiefel, J. S. Valentine, I. Bertini University Science Book; 2006
7. Reaction Mechanism of Inorganic and Organometallic Systems, R. B. Jordan, 2nd Edn., Oxford

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University press, 1991.
8. Bioinorganic Chemistry, A. K. Das, Allied Books, Kolkata, 2004.
9. Molecular Symmetry and Group Theory: A programmed Introduction to Chemical Applications, A. Vincent, John Wiley, 2001.
10. Mechanism of Inorganic Reactions, F. Basolo and R. G. Pearson, 2nd Edn. Wiley, 1967.

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C706: Advanced Organic Chemistry

Course Outcomes:

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

Course Details:

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

Recommended Books:

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

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C801: Heterocyclic and Natural Product Chemistry

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

Course Details:

1. *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.
2. *Chemistry of Natural Products*: Introduction and application of Carbohydrates; Steroids, Terpenoids, Fatty Lipids, Prostaglandins and alkaloid; Biogenesis and total synthesis of selected natural products.
3. *Chemistry of Biomolecules*: Classification and structures of amino acids; Peptides, Proteins and Nucleic acids; Solid phase synthesis; Nucleic acids synthesizer.

Recommended Books:

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.

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C802: Organometallic Chemistry

Course Outcomes:

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

Course Details:

1. General Properties of Organometallic Complexes: Werner Complexes; Trans Effect; Soft vs Hard Ligands; Crystal Field Theory; Back Bonding; Electroneutrality; Types of Ligands; 18-Electron Rule and Limitations; Electron Counting in Reactions; Oxidation State, Coordination Number and Geometry; Effects of Complexation; Difference between Metals; Outer Sphere Coordination.
2. Complexes with σ-Bonded Ligands: Transition Metal Alkyls and Aryls; Related σ-Bonded Ligands; Metal Hydride Complexes; σ-Complexes and Bond Strength; Metal Complexes of CO, RNC, CS, NO, Phosphine and Related Ligands.
3. Complexes with π-Bound Ligands: Alkene and Alkyl Complexes; Allyl Complexes; Diene Complexes; Cyclopentadienyl Complexes; Arenes and Other Alicyclic Ligands; Metalacycles; Polyene and Polyenyl Complexes.
4. Ligand Substitution, Oxidative Addition and Reductive Elimination: Dissociative Substitution; Associative Mechanism; Redox Effect; Rearrangement in Substitution; Photochemical Substitution; Concerted Addition; SN^2 Reaction; Radical Mechanism; Ionic Mechanism; Reductive Elimination; σ-Bond Metathesis; Oxidative Coupling and Reductive Cleavage.
5. Metal-Ligand Multiple Bonds: Carbenes; Carbynes; Bridging Carbenes and Carbynes; N-heterocyclic Carbenes; Multiple Bonds to Heteroatoms.
6. Application in Homogeneous Catalysis: Alkene Isomerization; Alkene Hydrogenation; Alkene Hydroformylation; Hydrocyanation; Alkene Hydrosilylation; Alkene Hydroboration; Coupling Reactions; Alkene Metathesis; Polymerization of Alkene.
7. *Application to Organic Synthesis*: C-H Activation; Metal Alkyls, Aryls and Hydrides; Reduction and Oxidation; Protection and Deprotection; Reductive Elimination; Coupling Reaction; Insertion Reaction; Nucleophilic Attack on a Ligand.

Recommended Books:

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

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C803: Applied Spectroscopy-I

Course Outcomes:

- To learn the 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.

Course Details:

1. Nuclear Magnetic Resonance Spectroscopy: Basic principles, Chemical shifts, Spin-spin interactions; Application of ^{1}H and ^{13}C NMR spectroscopy including NOE, COSY, NOESY, and other 2D techniques in the structure determination of bioorganic compounds; Application in conformational analysis. Multinuclear (^{31}P, ^{19}F, ^{29}Si) 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.
2. 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, VO^{2+} containing systems: g values; Symmetry; The practical interpretation of ESR spectra, In solid state and solution states; Multiple electron systems; Triplet ground state, Zero field splitting, Kramers degeneracy, Spectral line-shapes when D « hν, D ~hν and D » hν. EPR of photoexcited triplet states.
3. 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.
4. Mossbauer Spectroscopy: Basic physical concepts; Spectral line shape; Isomer shift; Quadrupole splitting, Magnetic hyperfine interaction; Interpretation of Moss-Bauer parameters of ^{57}Fe, ^{99}Ru, ^{101}Ru, ^{195}Pt,^{193}Ir and ^{110}Sn; Some special applications: Solid state reactions; Thermal decomposition, Ligand exchange, Electron transfer, Isomerism, Surface studies and biological applications.

Recommended Books:

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

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Hill, UK,1973.
7. Mossbauer Spectroscopy, N. N. Greenwood and T. C. Gibb, Chapman & Hall, 1971.
8. Electron Spin Resonance: Elementary Theory and Practical Applications, J. E. Wertz and J. R. Bolton, Mcgraw Hill, 1984.

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804: Applied Spectroscopy-II

Course Outcomes:

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

Course Details:

1. Ultraviolet Spectroscopy: Electronic Transition; Definitions of related terms and designation of UV- absorption band; Studies of conjugated and extended conjugated systems; Woodward-Fiesher rules; Analytical use of UV-spectroscopy.
2. 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.
3. Fluorescence Spectroscopy: Phenomena of fluorescence; Photochemical laws; General characteristics; Quantum yield and its measurements; Radiationless transitions; Spin states and their interconversion; Kasha's rule and solvent effect; Spin orbit coupling; Energy transfer processes; Donor acceptor complexes, Excimers and Exiplexes. Fluorescence quenching (static and dynamic); Stern Volmer analysis; Timescale of molecular processes in solution. Steady-state and time resolved fluorescence. Fluorescence anisotropy; Biochemical fluorophores; New fluorescence technologies: Multiphoton Excitation, Fluorescence correlation Spectroscopy, Single molecule detection.
4. Photoelectron Spectroscopy: Experimental methods, Ionisation processes and Koopmans theorem; Photoelectron spectra and their interpretation and applications.
5. Mass Spectrometry: Basic concepts; Instrumentation, Fragmentation and rearrangements (including McLafferty rearrangement) of different classes of organic molecules; Isotope effects.

Recommended Books:

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.

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

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7. Appendix B

All Laboratory Courses: 15 weeks (including exams), 4 lab classes (of three hours duration each) per week.

C741: Organic Chemistry Laboratory-I : Organic Synthesis and Analysis

Course Outcomes:

- To learn basic reaction techniques
- To preform air and moisture sensitive reactions such as Grignard, Friedel Craft reactions
- To learn characterization of organic molecules such as spectral and analytical data
- To perform mg to gram scale reactions

Course Details:

1. 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.
2. Synthesis of the following compounds using name reactions:
    a. Diels-alder reaction of anthracene and Maleic anhydride
    b. Synthesis of Cinnamic acid from Benzaldehyde (perkin reaction)
    c. Synthesis of Triphenyl Carbinol (Grignard Reaction)
    d. Synthesis of 2-hydroxy-5-methyl benzophenone (Fries rearrangement)
    e. Synthesis of Benzilic acid from Benzil (Benzil- Benzilic acid rearrangement)
    f. Synthesis of p-methoxycinnamic acid (Knoevenagel reaction).
3. Synthesis of Benzanilide from benzophenone oxime (Beckman rearrangement)
4. Synthesis of 2-phenylindole from acetophenone phenylhydrazone (Fischer-indole synthesis)
5. Protection and deprotection technique: Synthesis of a ketal of cyclohexanone with ethylene glycol and regeneration of the ketone from the intermediate.
6. Esterification of p-methoxycinnamic acid.
7. Preparation of o-benzoylbenzoic acid from phthalic anhydride and benzene. The following activities also will be included. Use of chemical data base (from Merck or CRC Handbook); use of ISIS/Chemdraw or any other software for drawing structures and indicating mechanisms; use of models for drawing various projections.

Recommended Books:

1. Vogels Textbook of Quantitative Chemical Analysis, G. H. Jeffery, J. Bassett, J. Mendham and R. C. Denny, 5th Edn., ELBS, 1991.
2. Spectrometric Identification of Organic Compounds, R. M. Silverstein, G. C. Bassler and T. C. Morrill, 6th Edn., Wiley, 1998.
3. A Collection of Interesting general Chemistry Experiments, Anil J. Elias, Universities Press, 2007.
4. Laboratory Manual of Organic Chemistry, B. B. Dey and M. V. Sitaraman, Allied Publishers, 1992.
5. Laboratory Manual of Organic Chemistry, R. K. Bansal, New Age International Publishers, 2006.

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C742: Inorganic Chemistry Laboratory-I

Course Outcomes:

- Learn synthesis, purification, extraction and recrystallization techniques along with various techniques for characterization viz. IR, UV-Vis Spectroscopy, CV (cyclic voltammetry), and magnetic susceptibilities.
- Learn preparation and use of ion exchange column which is used in pharmaceutical Industry.
- Able to clearly communicate the results of scientific work in oral, written and electronic formats to both scientists and the public at large

Course Details:

1. Synthesis of metal complexes: a) $Mn(acac)_3$ and Fe(salen)Cl complexes; b) Elucidation of Redox behavior of the Mn(iii) and Fe(iii); and c) Elucidation of magnetic properties
2. Preparation and characterization of (mesitylene) tricarbonyl molybdenum (0).: a) Synthesis and characterization of 2,6-bis(diphenylmethyl)-4-methylaniline; b) Synthesis and characterize compound N,N-bis(2,6-bis(diphenylmethyl) 4-methylphenyl) diazabutadiene.
3. Synthesis and characterization of the monoanionic and bidentate amidine ligand.: a) Synthesis of meso tetratolul porphyrin from pyrrole and p-tolualdehyde.; b) Synthesis and characterization of zinc-porphyrin (meso-tetratolyl porphyrin) complex.; Preparation of dimethyl ester of pyridine 2,6-dicarboxylic acid. b) Synthesis and Characterization of 7E n-(1-3(E- 1-(2,6-diisopropylphenylimino) ethyl) phenyl) ethylidene)2,6 diisopropyl- benzenamine
4. Separation of the chromium complexes by using ion exchange column.
5. Synthesis and study of Mn(iii) (Salen)Cl by Cyclic Voltammetry and Differential Pulse Voltammetry (DPV), and determination of the following: the formal reduction potential (Eo!); the number of electrons transferred in the redox process (n); the diffusion coefficient (D); electrochemical reversibility; and the effects of varying concentration (C) and scan rate.
6. Synthesis and analysis of nanoparticles by using Disc Centrifuge.
7. Preparation and determination of the effective magnetic moment and number of unpaired electrons in $Mn(acac)_3$.
8. Preparation and determination of the aquation rate of $[Co(NH_3)_5Cl]Cl_2$.
9. Preparation and resolution of the optically active compound $Co(en)^{3+}$.

Recommended Books:

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

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C743: Organic Chemistry Laboratory-II

Course Outcomes:

- Independent ability to set up a chemical reaction.
- Understanding the reaction progress and monitoring.
- Isolation and characterization of organic compounds

Course Details:

Multistep Synthesis of Organic Compounds and Characterization by Spectroscopic Techniques

1. Phenylacetylene from cinnamic acid (via dibromocinnamic acid and phenylpropiolic acid).
2. 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. Nitration, reduction and diazotization reaction: mhydroxyacetophenone from acetophenone (via mnitroacetophenone and aminoacetophenone).
4. Dimedone from acetone (via mesityl oxide).
5. 3-Hydroxycoumarin from glycine (via hippuric acid).
6. Quinoline-2-carboxylic acid from aniline (via 2-methylquinoline and ω- tribromo- quinalidine).
7. 2-aminobenzothiazole from aniline (via phenyl thiouea).
8. Synthesis of a drug (Uramil): aminobarbituric acid (Uramil) from diethylmalonate (via barbituric acid and nitro barbituric acid).
9. Beckmann Rearrangement: 6-Phenanthridone from fluorenone (via fluorenone oxime).
10. Synthesis of N, O-Heterocycle: 2,4,5-Triphenyloxazole from benzoin (via desylben- zoate).
11. 9-acridone from o-chlorobenzoic acid (via n-phenylanthranilic acid).
12. 3,4-Dihydro-4-oxo-1,2,3-benzotriazine from methyl anthranilate (via anthranilohy- drazide).
13. Synthesis of Mesoionic compound (p-Chlorophenylsydnone): p-Chlorophenylsydnone from p-chloroaniline (via n-p- chlorophenylglycine- ethyl ester, n-(p-chlorophenyl) glycine), and n-nitroso- n-(p-chlorophenyl) glycine.
14. Diastereoselective reduction of benzil.

Recommended Books:

1. Intermediates for Organic Synthesis, V. K. Ahluwalia, P. Bhagat, R. Aggarwal, R. Chandra, I. K. International, New Delhi, 2005.
2. Practical Heterocyclic Chemistry, A. O. Fitton and R. K. Smalley, Academic Press, London, 1968.

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C744: Physical Chemistry Laboratory

Course Outcomes:

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

Course Details:

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

Recommended Books:

1. Experiments in physical chemistry, 8th ed. / Carl W. Garland, Joseph W. Nibler, David P. Shoemaker, McGraw-Hill, 2009.
2. A Collection of Interesting General Chemistry Experiments, A. J. Elias, Universities Press, 2007.
3. Experimental Physical Chemistry: A Laboratory Text, 3rd ed. Arthur Halpern, George McBane, Publisher: W. H. Freeman; 2006.

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4. T. Engel and P. Reid, Physical Chemistry, Pearson, 2013.
5. P. W. Atkins and R. S. Friedmann, Molecular Quantum Mechanics, Oxford, 2008.
6. D. A. McQuarrie and J. D. Simon, Physical Chemistry – A Molecular Approach, Viva Books, New Delhi, 1998.

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C841: Inorganic Chemistry Laboratory-II

Course Outcomes:

- Familiarization with advanced techniques for syntheses and characterization of coordination compounds and organomatallic complexes including the use of standard Schlenk and vacuum line techniques.
- Crystallization, distillation and sublimation as purification methods will be practiced.
- Students will have learnt the use of various analytical and spectroscopic methods

Course Details:

1. Synthesis and reactivities of organocobaloximes.
2. Preparation of tris(acetylacetonato) iron(III).
3. Preparation tris(ethylenediammine)cobalt(II) ion and its resolution into optical antipodes.
4. Synthesis of hexaminecobalt(III) chloride and pentammineaquacobalt(III) chloride.
5. Preparation of an iron (or nickel) nitrosyl complex.
6. Synthesis of a cationic iodine complex.
7. Synthesis of bis(cyclopentadienyl)iron(II) (ferrocene).
8. Dilithiation of ferrocene and synthetic uses of the product in the preparation of acetyl ferrocene.
9. Preparation of bis(cyclopentadienyl) nickel (nickelocene).
10. Synthesis of a metal-metal bonded cyclopentadienyl complex of molybdenum, $Cp_2Mo_2(CO)_6$.
11. Synthesis of an arenetricarbonyl chromium(0) complex.
12. Preparation of boronic acid from Grignard reagents and trimethyl borate.
13. Preparation of chiral salen based catalysts of Co, Cr derived from 3,5-di-tert-butylsalicylaldehdye and trans-1,2-diaminocyclohexane

Recommended Books

i. J. D. Woollins, Inorganic Experiments, 2nd Ed, Wiley-VCH, Weinheim (2003).
ii. M. A. Malati, Experimental Inorganic/Physical Chemistry: An Investigative, Integrated Approach to Practical Project Work, Horwood Publishing Ltd, England (1999).
iii. J. Tanaka, S. L. Suib, Experimental Methods in Inorganic Chemistry, Prentice Hall, New Jersey (1999).

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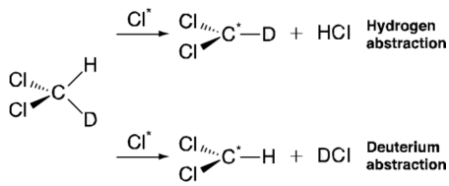
C842: Computational Chemistry Lab

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

Course Details:

1. Calculation of kinetic Isotope effects in chemical reactions using DFT methods.

Example: 

2. Simulated vibrational, rovibrational and rotational Raman Spectra for diatomic molecules using spreadsheet. Example: HCl, N2
3. Simulation of electronic spectra of simple molecules using CIS and TDDFT methods. Example: butadiene, hexatriene, and octatetraene
4. 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.
5. 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.
6. 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.
7. Study of the relationship between HOMO-LUMO energy gaps, energy barriers and rate constants in Diels-Alder reactions using DFT methods.
8. Study of the vibrational spectra protonated water cluster (dimer, trimer etc) and compare them with the experimental results such as Johnson's work. (Science, 299, 1375 (2003).
9. Activation energy, forward and backward rate constant and equilibrium constant for isomerization reactions to introduce Arrhenius equation and Eyring equation.
10. Study of thermodynamic properties of Lennard-Jones fluids from molecular dynamics simulations.
11. Application of Monte-Carlo simulations - Estimation of the value of π

Recommended Books:

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.

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C843: Research Laboratory

Contact: 6 hours/week

Course Outcomes**:**

This course is aimed to expose the students to the different research topics and research environments available in the School of Chemical Sciences. This will help students to decide their research area in which they would like to pursue for their Ph.D. In this course, the students are required to work in three research labs to gain exposure to the research field and the research environment on a rotation basis.

Each student will be needed to select THREE faculty members (PI) with whom he/she would like to carry out their lab rotation. The duration of each lab rotation is 4 WEEKS. The students are, however, not restricted to join one of these three research groups later for the project and/or the doctoral studies.

Schedule:

Lab rotation I: Week 1 to Week 4
Lab rotation II: Week 5 to Week 8
Lab rotation III: Week 9 to Week 12

Grading: Each faculty member will give their scores for the lab rotation for a maximum of 100 marks. The course coordinator will use the average of the marks for letter grades.

Activities during lab rotation:
During each rotation, students are expected to involve in various activities of the research group including:

- Schedule meetings with the PI to discuss research projects, expectations, mentoring style, etc.
- Read papers and/or submit assignments related to the research work as suggested by the PI
- Involve in research discussion with other group members
- Basic training of research instruments and protocols
- Basic training on experimental and/or computational research
- Develop basic scientific communication skills
- Attend group meetings and/or subgroup meetings
- Make a presentation to the PI and/or research group about their activities during the end of their rotation period

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Appendix C

Elective Courses (8 credit course)

C901: Photochemistry

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

Course Details:

1. 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).
2. Unimolecular Photophysical Processes: Jablonski Diagram; Frank-Condon principle; Fluorescence; Inter-System Crossing; Phosphorescence; Delayed Fluorescence; Quantum Yield.
3. 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.
4. 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.
5. Photochemistry of Organic Compounds: Photochemistry of alkenes; Pericyclic Reactions; Photo-oxidation and photo-reduction; Photochemistry of Carbonyl Compounds.
6. Applied Photochemistry: Chemistry of Vision; Photochemistry in nature; Photochemistry in atmosphere; Supramolecular photochemistry; Solar Cell; Fuel cell.

Recommended Books:

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

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C902: Pharmaceutical Chemistry

Course Outcomes:

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

Course Details:

1. 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.
2. 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.
3. Pharmacodynamics and pharmacokinetics: Drug distribution and survival; Concept of prodrug; Pharmacokinetic models; Drug metabolism.

Recommended Books:

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

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C903: Classics in Molecules

Course Outcomes:

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

Course Details:

1. Introduction, Understanding Structural Diagrams of Organic Molecules, Protein and Three-dimensional protein Structure, Nucleic acids, Synthesis, Biosynthesis.
2. 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,
3. Cyclosporin, FK506 & Rapamycin, Calicheamicin $\gamma 1$, Palytoxin, Taxol, Mevacor, Zaragozic acids & Cp Molecules, Brevetoxin B, Ecteinascidin 743, Epothilones, Resiniferatoxin, Vancomycin, Thiostrepton.
4. Modern Drug Discovery and Developments, Designed Small Drug Molecules for Mental illness, Viral infections, gastrointestinal Disorders, Heart diseases and Sexual Dysfunction.
5. DNA Technologies, Vaccines, antibodies, Diabetes, anemia, Rheumatoid arthritis, Breast Cancer, Biologics.

Recommended Books:

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.

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C904: Molecular Modeling

Course Outcomes:

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

Course Details:

1. Introduction: What is molecular modeling? Computable quantities.
2. Concept of Potential Energy Surface: Stationary points, Born-Oppenheimer approximation, Geometry optimization, Normal modes of vibration.
3. Molecular Mechanics: Basic principles, properties that can be calculated, Strengths and weaknesses.
4. Quantum Mechanics: Hartree-Fock-Self-Consistent-Field theory, Post-Hartree- Fock (Electron correlation) methods, Density functional theory, Semi-empirical methods.
2. Chemical Dynamics: Unimolecular and Bimolecular reactions, Reaction path and transition states, Classical trajectories, Direct dynamics, Quantum dynamics.
3. Simulations of Molecular Ensembles: Properties as ensemble and time averages, Molecular dynamics simulations, Monte Carlo simulations.
4. Modeling Lab: Hands-on experience for using different simulations methods and algorithms pertaining to the course.

Recommended Books:

1. C. J. Cramer, Essentials of Computational Chemistry, Wiley, 2004.
2. 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.

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C905: Solid State Chemistry

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

Course Details:

1. 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 & nonmetallic structures, AB, AB2, AB3 (ReO3), spinels, pyrochlores, perovskites, K2niF4 etc. paulings rules for ionic crystal structures and the concept of bond valence. Methods of crystallography: powder, single crystals, X-ray, neutron and electron diffraction.
2. 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.
3. 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.
4. Critical Phenomena: Phase transitions (Order-disorder, Martensite-austenite, Spinoidal 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.

2. 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.
3. Superconductivity: Superconductivity: General aspects of superconductivity; Effects of magnetic field; BCS Theory; Oxide Superconductors.

Recommended Books:

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.

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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.

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C906: Crystallography

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

Course Details:

1. Origin of X-rays, Filters, Monochromators, Sealed tube, Rotating anode synchroton radiation, Safety considerations.
2. Crystals and their properties- Concepts of symmetry, Direct and reciprocal lattice, Planes, Indices, Unit cell, Braggs 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.
3. 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 patters on and direct methods.
4. 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.

Recommended Books:

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.

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C907: Principles of Drug Action

Course Outcomes:

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

Course Details:

1. 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.
2. 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.
3. 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.
4. 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.
5. 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 ageing and hydrolysis, Other mechanisms of degradation.
6. Drug Development: Clinical trials (Phase-I to phase-IV), Formulation development, Quality control aspects (methods of assay).

Recommended Books:

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.

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C908: Advanced Bio-inorganic Chemistry

Course Outcomes:

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

Course Details:

1. Principles of bioinorganic Chemistry (Justification of why certain protein/enzyme contains a particular metal ion)
2. 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.
3. Iron-Sulfur Proteins: Types, function and mechanisms, Rubredoxin, Ferredoxins, Aconitase
2. Non-Heme Proteins: Types, function and mechanisms, Mononuclear Systems (Catechol-1,2-Dioxygenases, Transferrin, Ferritin, Superoxide Dismutase, Isopenicillinn- Synthase) Dinuclear Systems (Hemerythrin, Ribonucleotide Reductase, Methane Monooxygenase, Purple acid phosphatases)
3. Copper Proteins (Type i, ii, and iii): Types, function and mechanisms, Blue Copper proteins; Hemocyanin, Tyrosinase, Catechol Oxidase; Superoxide Dismutase; ascorbase Oxidase, Laccase; galactose oxidase
4. Molybdenum Enzymes: Types, function and mechanisms, Oxo-Transfer Enzymes, Xanthine Oxidase, Nitrogenase.
5. Manganese: Photosynthesis (Photosystem I and Photosystem II); function and mechanisms.
6. Zinc Enzymes: Function and mechanisms, Hydrolytic Enzymes (Carbonic anhydrase; Carboxy peptidase A; Alkaline phosphatase).
7. DNA/RNA: Types, function and mechanisms, DNA nicking enzymes; DNA polymerase; Ribozymes.

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8. Environmental & Medicinal Aspects: Acid-rain; Green-house Effect etc. Radiopharmaceuticals; Photo-Dynamic Therapy; Anti-Tumor Drugs (cis-platin, Carboplatin; Bleomycins); Ion-pumps.

Recommended Books:

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 Internet.

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C909: Nuclear Magnetic Resonance

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.

Course Details:

1. Classical NMR Spectroscopy: Nuclear magnetism, Bloch equations, Chemical shift, Linewidth, Scalar coupling
2. 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.
3. 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 transer protocols like in EpT.
4. 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 NMR experiment.
5. Two-dimensional NMR Experiments: Two-dimensional spectroscopy, Coherence transfer, COSY, double quantum filtered COSY, TOCSY, NOESY, HSQC, HMQC, Sensitivity enhanced HSQC.
6. 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.

Recommended Books:

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.

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C910: Advanced Functional materials

Course Outcomes:

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

Course Details:

1. Introduction to Materials in Modern Technology: Materials as an enabling element of technological progress; Functions that materials perform; The properties - structure - processing connection.
2. 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.
3. Dielectric Materials: Dielectric constant and polarizability, Insulating materials, Ferroelectrics, piezo electrics, Measurement of Dielectric properties, Applications.
2. Nanosized Magnetic Materials: Basic concepts of magnetism; Types of magnetic behavior, Magnetic domains, Soft and hard magnets, Classification magnetic nanomaterials, Ferrofluids, Single-domain particles, Physical Properties of Magnetic nanostructures, Nano magnetism for biological applications.
3. Polymer Materials and Nano-composites: Classification of Polymers, Structure- Property Correlation, Molecular weights, Conduction in polymers, Natural composities, 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.
4. Amorphous and Crystalline Porous Materials: Crystalline vs. Amorphous Solids, Glass Formation, Structural models of amorphous materials, Properties of metaglasses, Evolution and Development of porous materials, Chemistry of microporous materials, Mesoporous materials, Semiconductor nanoparticles in Zeolites, Polymers and carbon materials in Zeolites.

Recommended Books:

1. Fundamental 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.

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C911: Supramolecular Chemistry

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

Course Details:

1. Introduction: Understanding of Supramolecular Chemistry (Multidisciplinary nature, Complementarities in biology); Selectivity; Supramolecular interactions; Chelate and Macrocyclic Effects; Characterizing Supramolecular Systems; Structural, Kinetic and Thermodynamic.
2. Molecular Self-assembly: Non-Covalent Interactions: Electrostatic, Hydrogen Bonding, $\pi - \pi$ 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.
3. Synthesis of Macrocycles: High Dilution Technique; Coordination Template Effects; Cation Binding and De-Metallation; Porphyrins; Corrins; Crown Ethers; Cryptands; Spherands; Sepulchrates; Siderophores; Calixarenes.
2. 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.

Recommended Books:

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

Reference styles to be uniform

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C912: Chemistry of Nanomaterials

Course Outcomes:

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

Course Details:

1. Introduction: Nano and nature, Fascination and Motivation of nanoparticle research, Bottom-up and Top-down approaches.
2. Zero and One-Dimensional Nano Structures: 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.
3. Carbon Nanomaterials: Fullerenes and their Derivatives, Carbon nanotubes: Structure and properties, nanocrystalline Diamond.
4. Self-assembled Monolayers: Introduction, Monolayers on gold, Growth process, Phase transitions, Patterning monolyers, Mixed monolayers structure, Electrochemistry and applications of self- assembled monolayers of thiols.
5. Nano and Micro-emulsion: Surface active agents, Micellization, Mechanism of emulsion, Characterization of Microemulsion.
6. Application of Nanomaterials: Solar energy conversion, Molecular and nano- electronics, Nanocatalysis, Biological applications and other applications.

Recommended Books:

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, 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 Yurygogotsi, Taylor and Francis Group, LLC, 2006.
5. Carbon Nanotubes and Related Structures, Edited by Dirk M. Guldi and Nazario Mart´ın, 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.

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C913: Advanced Bioorganic Chemistry

Course Outcomes:

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

Course Details:

1. Enzymology: Mechanistic studies of enzymatic reactions. Studies of enzyme kinetic 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 Retroreactions; Formylations, Hydroxy methylations, and Methylations; rearrangements.
2. Application of Enzyme Kinetics: Substrate Kinetics; Kinetics of Enzyme inhibition; Substrate inhibition; Non-productive Binding; Competing Substrates; Multi- substrate Systems; Allosterism and Cooperativity.
3. 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.
4. 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).
5. Introduction of Vital Bio-macromolecule Secondary Structures: g-Quadruplex, i-motif, RNAi (mi-RNA &si-RNA) & Collagen and their application in therapeutics.

Recommended Books:

1. Organic Chemistry of Enzyme-Catalyzed Reactions, Revised Edition by Richard Silverman published: FEB-2002. ISBN 10: 0-12-643731-9, Academic Press.
2. Structure and Mechanism in Protein Science: A Guide to Enzyme Catalysis and Protein Folding ByalanFersht, Publisher: W. H. Freeman; 1st Edn. (September 15, 1998)
3. Evaluation of Enzyme Inhibitors in Drug Discovery: A Guide for Medicinal Chemists and Pharmacologists (Methods of Biochemical analysis); by Robert A. Copeland, Publisher: Wiley-interscience; 1st Edn. (March 28, 2005).
4. Dewick, Paul M. Medicinal Natural Products: A Biosynthetic Approach. 2nd Edn.. New York, NY: John Wiley & Sons, inc.,2001. ISBN: 9780471496410 (paperback).
5. Structural Diversity of g-Quadruplex Scaffolds; Stephen Neidle and Shankar Balasubramanian, CRC Press Copyright Year-2006.

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6. Gene Silencing by RNA Interference: Technology and Application, by Muhammad Sohail (Editor), CRC Press; 1st Edn. (July 26, 2004).
7. Modified Nucleosides: in Biochemistry, Biotechnology and Medicine (ed P. Herdewijn), Wiley-VCH Verlag GmbH &Co. Kgaa, Weinheim, Germany.
8. Natural products: The Secondary Metabolites, James R. Hanson Copyright Year:2003. ISBN: 978-1- 84755-153-5

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C914: Polymer Chemistry

Course Outcomes:

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

Course Details:

1. 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.
2. 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.
3. Kinetics of polymerization, Free-radical, Cationic and Anionic polymerization and polycondensation.
4. Copolymerization, Free-radical and ionic copolymerization and Copolycondensation.
5. 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.
6. Biodegradable polymers: Synthesis and challenges.

Recommended Books:

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.

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C915: Molecular Reaction Dynamics

Course Outcomes:

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

Course Details:

1. Introduction: The rate constant - History and current view. What is molecular reaction dynamics.
2. Theoretical methods i: Transition State Theory (TST), RRKM Theory.
3. Theoretical Methods ii: Rate and cross-section, Classical scattering theory, Quantum scattering theory (reactive and non- reactive), Connection to TST and RRKM.
4. Experimental methods: Newton's diagrams, Molecular Beams, State-resolved spectroscopic techniques, Imaging techniques.
5. Applications: Photoselective chemistry - photodissociation and photoisomerization dynamics, Dynamics in real-time (ps, fs and attosecond regimes), Molecular energy transfer, Control of chemical reactions. Dynamics of gas-surface reactions.
6. Condensed phase dynamics, Solvation dynamics.

Recommended Books:

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

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C916: Theory of Molecular 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

Course Details:

1. Recap: Introduction and review of basic quantum mechanics, Molecular symmetry.
2. Rovibronic Hamiltonian - Coordinates and Momenta: Euler angles, Axis systems, Rotational and vibrational angular momentum, Normal and internal coordinates, the g matrix, the gF matrix.
3. Rovibronic Wavefunctions: Classification of rotational, Vibrational, Rotation-Vibration, and electronic wave functions, Hund's cases.
4. Energy Levels and Interaction: Rotation-vibration interactions, Vibronic and rovibronic interactions, Renner-Teller and Jahn-Teller effect, Rydberg states, Spin effects.
5. Transition intensities and optical selection rules, Electric - magnetic dipole and electric quadrupole transitions, Multiphoton processes and Raman effect.
6. Advanced topics: Spectroscopy at high energies, Intramolecular vibrational energy redistribution (IVR), Wave-packet approach to spectroscopy.

Recommended Books:

1. P. R. Bunker and P. Jensen, Molecular Symmetry and Spectroscopy, NRC Research Press, Ottawa. (1999)
2. J. D. Graybeal, Molecular Spectroscopy, Mcgraw-Hill. (1988) Year to be written in 1 and 2 refs
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.

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C918: Catalysis: Reaction Mechanisms and Applications

Course Outcomes:

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

Course Details:

1. Introduction to Catalysis: Fundamental concepts.
2. Survey of Ligands: Characteristics of the transition-metal in the complexes; Elementary steps.
3. Reaction Mechanisms and Applications: Carbonylation, Hydroformylation, Hydrogenation, metathesis reactions, Oxidation reactions, Isomerization reactions, Cross- Coupling reactions, and C- H functionalization reactions.
4. Examples of synthetic and industrial applications.

Recommended Books:

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.

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C919: Advanced Main Group Chemistry

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

Course Details:

1. (a) 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.
2. N-heterocyclic carbene (NHC) stabilized low oxidation state main group metal complexes.
3. Low Oxidation State Main Group Metal Hydrides: Synthesis and reactivity.
4. N-heterocyclic carbenes (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) Hetero cylces.
5. Role of main group compounds in catalysis, Organic synthesis and medicinal chemistry
6. Inorganic New Materials: Nanomaterials, Polymers and chemical sensors.

(Should we use the full form of NHC and define the abbreviation)

Recommended Books:

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.

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C920: Advanced Fluorescence Spectroscopy

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 biological related molecules
- It also introduces fluorescence imaging

Course Details:

1. 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.
2. 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.
3. 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.
4. 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. Electron transfer reactions and Marcus theory.
5. Multiphoton Excitation: Introduction to Multiphoton Excitation, Two-photon Absorption Spectra, Cross Section for Multi-photon Absorption.
6. Single-molecule Detection (SmD): Detectability of Single Molecules, Instrumentation for SMD, Single-Molecule photophysics, Biochemical applications of SMD.
7. Fluorescence Correlation Spectroscopy (FCS): Principles of Fluorescence Correlation Spectroscopy, Theory of FCS, Examples of FCS Experiments.
8. Fluorescence-Lifetime imaging microscopy (FLim): Early Methods for Fluorescence- Lifetime imaging, Laser Scanning TCSpCFLiM, Lifetime imaging of Cellular Biomolecules.
9. 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.

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Recommended Books:

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.

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C921: Biomacromolecules

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

Course Details:

1. Buffers (their use in study of biomolecules), pH, pKa of amino acids, D and L amino acid nomenclature.
2. 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.
3. 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.
4. 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).
5. Carbohydrates and glycoproteins, Proteoglycans, Membranes and lipids, Bacterial cell wall synthesis and mechanism of some important antibiotics like Penicillin, Antibiotic resistance.
6. Metabolism: Photosynthesis, Calvins cycle, Glycolysis, Krebs cycle, Electron transport, Cofactors.

Recommended Books:

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.

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C922: Advanced Heterocyclic Chemistry

Course Outcomes:

- Introduction of Heterocyclic Chemistry: Nomenclature, spectral characteristics, reactivity and aromaticity of heterocyles (three and four membered)
- Synthesis and reactivity of five membered rings, benzofused 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

Course Details:

1. Heterocyclic Chemistry; Introduction to heterocycles: Nomenclature, Spectral characteristics, Reactivity and Aromaticity.
2. Synthesis and reactivity of three and four membered heterocycles e.g., Aziridine, Azirine, Azetidine, Oxiranes, Thiarines, Oxetenes and Thietanes.
3. Synthesis and reactivity of five membered rings with two heteroatoms: Pyrazole, Imidazole, Oxazole, Thiazole, Isothiazole and Benzofused analogs; Benzofused five membered heterocycles with one heteroatom, e.g., Indole, Benzofuran, Benzothiophene.
4. Synthesis and reactivity of benzofused six membered rings with one, two and three heteroatoms: Benzopyrans, Quinolines, Isoquinoline, Quinoxazaline, Acridine, Phenoxazine, Phenothiazine, Benzotriazine, Pteridines.
5. Synthesis and reactivity of seven and large membered heterocycles: Azepines, Oxepines, Thiepines; Spiroheterocycles; Bicyclic compounds containing one or more heteroatoms
6. Recent methods of C-H functionalization/activations of heterocyclic derivatives.

Recommended Books:

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. (1995)
4. Advances in Heterocyclic Chemistry, Book Series Elsevier Edited by Alan Katritzky. 1997
5. Branden C and Tooze J., Introduction to Protein Structure, 2nd Edn., 1999.

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C923: Statistical Mechanics

Course Outcomes:

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

Course Details:

1. 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.
2. Calculations of partition functions and thermodynamic properties for ideal systems of monatomic and diatomic molecules.
3. Calculations of fluctuations and showing the equivalence of ensembles.
4. Calculation of heat capacity of solids, Einstein and Debye theories,
5. Study of chemical equilibrium, Equilibrium constantexpression in terms of partition functions.
6. Quantum Statistics: ~~Maxwell-Boltzmann~~, Bose-Einstein, and Fermi-Dirac statistics(compare with classical Maxwell-Boltzmann statistics). Systems of Fermions and Bosons in weak and strong degenerate limits.
7. Classical Statistical Mechanics: partition functions as integrals over phase space coordinates, Systems of interacting particles, imperfect gases, Concept of reduced distribution functions, concept of radial distribution functions of liquids and applications to ionic solutions using Debye-Huckel theory.
8. Non-equilibrium Statistical Mechanics: Onsager regression hypothesis and fluctuation-dissipation theorem, Calculations of transport coefficients like Diffusion, Conductivity.

   (Ordering is slightly changed as shown in red)

Recommended Books:

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.
6. T.L. Hill, An Introduction to Statistical Thermodynamics: Dover Publ., New York,1987

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C924: Frontiers in Organic Synthesis

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

Course Details:

1. Developing facets of organic synthesis
2. Domino Reactions: History, Definition, Classifications, Biological systems, Enantioselective reactions and Application in total synthesis
3. Non-activated C–H Functionalization: Mode of activation, Metal and Organocatalysts, Traceless organic synthesis, Decarboxylative cross-coupling reactions, Remote C-H functionalization, Recent examples
4. Protecting Group Free Total Synthesis: Historical context, Protection and Deprotection, Chemoselectivity, Recent advances in protecting groups free total synthesis
5. Recent Applications: Click Chemistry, Mechanochemistry, Photocatalysis

Recommended Books

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. Journals articles and Reviews

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