

Syllabus for PhD Elective Courses

Department of Chemistry, Indian Institute of Technology Guwahati

Even Semester (Jan-May)

CH7051

Bioinorganic Chemistry

3 -0 -0 -6

Prerequisite: Nil

Role of metal ions in Biology: Physiological effects of the presence or absence of metal ions in biology. Role of ions in respiration, metabolism, photosynthesis and gene regulation in brief. Hard-Soft Acid-Base Concept, chelate effect, pK_a values of the coordinated ligand, redox potential, Nernst equation, and kinetic aspects such as ligand exchange rate, substitution reactions, and electron transfer reactions. Brief description of peptide bond, primary, secondary and tertiary structure and hydrogen bonding. Various spectroscopic methods used in bioinorganic chemistry: Infrared, electronic spectra (especially d-d transitions), EPR (emphasis on first row transition metal ions and their spectra), a brief description of CD/MCD and multinuclear NMR. Brief description and capability of newer methods like EXAFS, XANES, ENDOR. Classifications of metalloproteins and enzymes based on function, with examples: Metalloproteins; Dioxygen transport (Hemoglobin, Hemocyanin), electron transfer (blue copper proteins, cytochromes, iron-sulphur proteins), structural roles (zinc finger), uptake and storage proteins (ferritins). Metalloenzymes: Hydrolytic enzymes (zinc enzymes), redox enzymes (Binuclear redox enzymes, SODs, photosystem II), oxygen-atom-transfer reactions (methane monooxygenase, catechol dioxygenase). Metalloproteins or enzymes, either newly discovered or of current research interest, not covered above, should be included. Discussion about different approaches employed in solving the problems in bioinorganic chemistry: Use of coordination complexes as a model. Models for various enzymes will be discussed along with the above-mentioned enzymes/proteins. Brief descriptions of other approaches like use of mutant enzymes. Topics of current interest: Thrust areas of research in bioinorganic chemistry, such as the role of nitric oxide and other topics, will be discussed, and students will participate in writing a short report on one such topic and discuss in class.

Text book:

1. S. J. Lippard and J. M. Berg, Principles of Bioinorganic Chemistry, University Science Books, Mill Valley, California. (Other journal articles and books will be referenced during the course.)

CH7052:

New Reagents for Organic Synthesis

3 -0 -0 6

Pre-requisites: Nil

Lanthanides in Organic Synthesis: General properties of Lanthanides. use of Lanthanide metal compounds at different oxidation states in synthesis. Reagents from (i) Cerium (ii) Samarium (iii) Ytterbium etc. Organotransition metal reagents: Principles, reagents developed from Titanium, Chromium, Iron, Rhodium, Nickel, Palladium. Reagents containing Phosphorous, Sulphur, Silicon or Boron: Introduction, Phosphorous-containing reagents, Sulphur-containing

reagents, Silicon-containing reagents, Boron-containing reagents. Oxidising reagents: Use of reagents such as Pyridinium Chloro Chromate, Pyridinium Fluoro Chromate, Swern oxidation, DCC oxidation, Tetrapropyl ammonium peruthenate, other oxidizing agents. Reducing agents: Reductions involving NaBH_4 , LiAlH_4 , NaBH_3CN , DIBAL-H, and Red-Al.

Texts:

1. R. O. C Norman and J. H. Coxon, Principles of Organic Synthesis, 1st Ed, ELBS, 1993.
2. T. Imamoto, Lanthanides in Organic Synthesis, Academic Press, 1994.
3. W. Carruther, Some Modern Methods of Organic Synthesis, Cambridge, 1990.
4. L. W. Paquette (Ed), Reagents for Organic Synthesis, John Wiley, 1995.

CH7053

Advances in Bio-Organic Chemistry

3-0-0-6

Pre-requisites: Basic knowledge in Biological Macromolecules/Biochemistry

Introduction to bioorganic chemistry; biomimetic chemistry; chemical biology: proteomics, glycomics, protein's secondary structures; peptidomimetics; peptide based drugs; recent trend in expanding genetic code; enzymes catalysis; drug targets: types, enzyme as drug target, inhibition and drug design, enzyme catalyzed reactions; antibody: catalytic antibodies, hapten design, examples of antibody catalyzed reactions; biomimetic polyene cyclisation; squalene biosynthesis; drug DNA interaction; RNAzymes; genetic alphabets; DNA detection-single nucleotide polymorphism (SNPs); human genome project; hap map project; gene therapy; human variome project; 1000 genomes project; personalized medicine.

Textbooks:

1. Lehninger Principles of Biochemistry, 5th Ed. by Nelson and Cox.
2. Hermann Dugas: Bioorganic Chemistry: A Chemical Approach to Enzyme Action; 3rd Edition.
3. The organic chemistry of enzyme-catalyzed reactions, by Richard B. Silverman, Academic Press, San Diego, 2000, 717 pp.

References:

1. Biochemistry, 5th Ed. (Hardcover) by Lubert Stryer, Jeremy M. Berg, and John L. Tymoczko.
2. NPTEL-Web-based Course, Bio-Organic Chemistry by S. S. Bag. Website: <https://nptel.ac.in/courses/104103018>.
3. Amino acids, peptides and proteins, by J. S. Davies, Royal Society of Chemistry, UK, Vol. 35, 2006.
4. Proteins, Enzymes, Genes: The Interplay of Chemistry and Biology by J.S. Fruton, Yale University Press, 1999. (xii + 783 pages).

CH7054

Organometallics

3 -0 -0 -6

Prerequisite: Nil

Definition, classifications and bonding in organometallics, isolobal analogies, structural aspects of organometallics, and preparative methods. Spectroscopic techniques in organometallic chemistry. Electronic and magnetic properties of organometallic compounds. Stoichiometric and catalytic reactions: Fundamental processes in reactions of organotransition metal complexes. Application of transition metal complexes to catalysis. Organometallics directed towards organic synthesis. Bio-organometallics, organometallics in environmental chemistry. Metal clusters and models for heterogeneous catalysis. Application of organometallics in industry.

Textbooks:

1. Yamamoto, Organotransition metal in Chemistry, Fundamental concept and applications; John Wiley, 1986.
2. R. H. Crabtree, The organometallic Chemistry of the transition metals, John Wiley, 1994.

CH7055: Advances in Biological Macromolecules

3-0-0-6

Pre-Requisites: Nil

Advances in proteins, solid phase peptide synthesis, synthesis of peptide antibiotics, posttranslational modification; advances in carbohydrates, oligosaccharides; lipids -fatty acids, bilayer, lipidation of proteins and peptides, farnesylation of the ras protein; biological membranes, transport across membranes, model membrane, insertion of lipidated peptides into model membrane and their biophysical properties, concepts of fluorescence and fluorescence markers, synthesis of vesicles containing fluorescence quencher and lipidated peptides; advances in nucleic acids-DNA replication, genetic information storage, transmission and gene expression, chemical synthesis of oligonucleotides, hybridization with synthetic oligonucleotides, nucleic acids as molecular probes, peptide nucleic acids (PNAs) synthesis, doubly labeled PNAs as probes for the detection of point mutations; use of small molecules to link a protein target to a cellular phenotype and as probes for biological processes.

Textbooks:

1. A. Miller and J. Tanner, Essentials of Chemical Biology, Wiley & Sons Ltd., 2008.
2. C.M. Dobson, J.A. Gerrard and A.J. Pratt, Foundations of Chemical biology, Oxford Univ. Press. 2002.
3. J. M. Berg, L. Tymoczko and L. Stryer. Biochemistry, W. H. Freeman and Company, New York.
4. Lehninger, Nelson and Cox, Principles of Biochemistry, CBS Publishers, 1993.

References:

1. S.L. Schreiber, T. Kapoor and G. W. Wiley Chemical Biology: from small molecules to systems biology and drug design, Vol. 1, VCH Verlag GmbH & Co. 2007.
2. B. Larijani, C. A. Rosser and R. Woscholski Chemical Biology: Application and Techniques, John Wiley & Sons Ltd. England, 2006.
3. H. Waldmann and P. Janning. Wiley Chemical Biology: A practical course, VCH Verlag GmbH & Co., 2004.
4. C.M. Dobson, J.A. Gerrard and A.J. Pratt., Foundations of Chemical biology, Oxford

University Press, 2002.

5. A. Miller and J. Tanner, Essentials of Chemical Biology, Wiley & Sons Ltd., 2008.

6. L. Stryer, J.M. Berg and J. L. Tymoczko, Biochemistry, 5th Ed. (Hardcover) 2002.

7. J. S. Davies, Amino acids, peptides and proteins Vol. 35, Royal Society of Chemistry, UK, 2006.

8. J.S. Futon, Proteins, Enzymes, Genes: The Interplay of Chemistry and Biology, (xii 1-783 pages). Yale University Press, 1999.

CH7056

Time Dependent Quantum Mechanics

3 -0 -0 6

Prerequisite: M.Sc. Chemistry or Physics.

Introduction; mathematical review; evolution operator: The Schrodinger, Heisenberg and interaction pictures; perturbation theory: Fermi's Golden Rule; numerical methods for wave packet representation and propagation: The Fourier grid, discrete variable representation, finite difference, split operator, Chebychev, Lanczos and the t,t' method; wave packet dynamics in harmonic oscillator; wavefunction auto-correlation: electronic wavefunction calculation, molecular spectra; two level system: Rabi oscillations; quantum tunneling: resonances; laser matter interaction: dipole approximation and the center of mass transformation, Gauge transformation, multiphoton interactions, above threshold ionization and dissociation, high harmonic generation, control of molecular dynamics, laser cooling and trapping.

Texts books:

1. M. H. Mittleman, Introduction to the Theory of Laser-Atom Interactions, 2nd Ed., Plenum US, 1993

2. G. C. Schatz and M. A. Ratner, Quantum Mechanics in Chemistry, Dover Publications, 2002.

3. S. A. Rice, and M. Zhao, Optical Control of Molecular Dynamics 1st Ed., Wiley-Interscience, 2000.

References:

1. N.B. Delone, and V.P. Krainov, Multiphoton Processes in Atoms, Springer Series on Atoms and Plasmas, Vol 13, Springer, 1994.

2. A. Szabo, and N. S. Ostlund, Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory, Dover Publications, 1996.

3. H. J. Metcalf, and P. van der Straten, Laser Cooling and Trapping 1st Ed., Springer, 2001

Odd Semester (Jul-Nov)

CH7151

Physical Methods in Chemistry

3 -0 -0 6

Prerequisite: Nil

Nuclear magnetic resonance spectroscopy: General principles, sensitivity of the method. CW and FTNMR, instrumentation. Application in chemical analysis (with special reference to ¹H NMR): Chemical shift, spin-spin splitting, area of peak, shift reagents, off-resonance decoupling,

nuclear Overhauser effect, selective population inversion, inter-nuclear double resonance (INDOR). Two-dimensional and three-dimensional NMR spectroscopies, solid-state and gas-phase NMR spectra, polarization transfer techniques. Infrared spectroscopy: Principles, factors influencing vibrational frequencies, preparation of samples, the range of IR radiation, and selection rules. Instrumentation: Representation of spectra, dispersive and Fourier-transform IR-spectroscopies. Application of IR spectroscopy to inorganic and organic compounds. Raman Spectroscopy: Principles, normal, resonance and laser Raman spectroscopies. Structure determination by symmetry selection rules (normal coordinate analysis). Application of Raman spectroscopy to structural chemistry. Electronic spectroscopy: General principles, electronic absorption by molecules, absorption peaks and molar absorptivity, absorption and intensity shifts. Selection rules and their implications. Analytical applications: qualitative and quantitative analyses. Electronic spectra of inorganic and organic compounds. Mass spectrometry: Principles, advantages and limitations of mass spectrometry; instrumentation, methods of ionization, metastable ions. Theory of mass spectrometry, structure elucidation of inorganic and organic compounds. Mossbauer spectroscopy: The Mossbauer effect, the Mossbauer nuclei, chemical isomer shift, quadrupole splitting, magnetic hyperfine interaction. Elucidation of the electronic structure of ^{57}Fe , ^{119}Sn etc. compounds using Mossbauer data; Mossbauer of biological systems. Chromatography: General principles, different types of chromatographic techniques, characteristics of working components and analytes. Normal phase and reverse phase chromatography. Efficiency and resolution: Theoretical plate concept, Van Deemter equation. Gas Chromatography: types of GC, basic components of GC, optimization of the method, GC-MS, and applications. High-performance Liquid Chromatography: Different types of HPLC, basic components of HPLC, optimization of methods, and applications. Electrochromatography: Principles and applications. Thermal Analysis: General principles of thermal analysis. Thermogravimetric Analysis (TGA): Principles, instrumentation, study of thermogram, applications, limitations, DTG, Chemical Vapor Deposition (CVD), Metal Oxide Vapor Deposition (MOVD). Differential Thermal Analysis (DTA): Principles, instrumentation, study of thermogram, applications and limitations. Differential Scanning Calorimetry (DSC): Principles, instrumentation, study of thermogram, applications and limitations. Cyclic Voltammetry and Coulometry: Basic principles and applications to the study of electroactive species.

References:

1. R. M. Silverstein, G. Clayton Bassler and C. Morrill, *Spectrometric Identification of Organic Compounds*, 5th Ed., John Wiley & Sons, 1991.
2. W. Kemp, *Organic spectroscopy*, 3rd Ed., ELBS, 1991.
3. R. S. Drago, *Physical Methods for Chemists*, 2nd Ed., Saunders College Publishing, 1992.
4. W. Kemp, *NMR in Chemistry: A Multinuclear Introduction*, Macmillan, 1986.
5. A. B. P. Lever, *Inorganic Electronic Spectroscopy*, 2nd Ed., Elsevier, 1986.
6. K. Nakamoto, *Infrared and Raman Spectra of Inorganic and Coordination Compounds*, Part A & B, John Wiley and Sons Inc., 5th Ed., 1997.
7. E. A. V. D. Ebsworth, D. W. H. Rankin and S. Cradock, *Structural Methods in Inorganic Chemistry*, 2nd Ed., Blackwell, 1991.

Pre-requisites: Nil

Retrosynthetic Analysis: Basic for retrosynthetic analysis, Transforms and retrons, Types of Transforms, Biomimetic Approach to Retrosynthesis, Chemical degradation as a tool for retrosynthesis, Chiron approach. Transform-Based Strategies: Transform guided retrosynthetic search, Diels-Alder cycloaddition as a T -goal, Retrosynthetic analysis by computer under T -goal guidance, Enantioselective transforms as T-goals, Mechanistic transform application, T-goal search using a tactical combination of transforms. Structure-Based and Topological Strategies: Structure-goal (S-goal) strategies, Acyclic strategies, disconnections, Ring-bond disconnections-isolated rings, Disconnection of fused-ring systems, Disconnection of bridged-ring systems. Stereochemical Strategies: Stereochemical simplification-transform stereoselectivity, Stereochemical complexity- clearable stereocenters, Stereochemical strategies-polycyclic systems, Stereochemical strategies acyclic systems. Functional Group-Based and other Strategies: Functional Group interconversion, functional group-keyed skeletal disconnections, disconnection using tactical sets of Functional Group-keyed transforms, Strategies use of Functional Group equivalents, Acyclic core group equivalents of cyclic Functional Groups, Functional Group-keyed removal of functional and stereocenters, Functional Group and appendages as keys for connective transforms. Use of Several Strategies: Multistrategic retrosynthetic Analysis of longifolene, parontherine, perhydrohistrionicotoxin, Gibberellic acid, Picrotoxinin.

Texts:

1. E. J. Corey and Xue-Min Cheng, The logic of chemical synthesis, John Wiley, 1989.
2. M. B. Smith, Organic synthesis, McGraw-Hill Inc, New York, 1994.
3. Stuart Warren and Paul Wyatt, Organic Synthesis: The Disconnection Approach, Wiley; 2nd edition, 2008.

Prerequisite: Nil

Definitions and Theorems of Group Theory: Properties of Group and examples, subgroups, classes. Molecular Symmetry and the Symmetry Groups: Symmetry elements and operations: symmetry planes and reflections, the inversion Center, proper axes and proper rotation, and improper axes and improper rotations, products of symmetry operations, equivalent symmetry elements and equivalent atoms, General relations among symmetry elements and operations, Symmetry elements and optical isomerism, symmetry point groups, symmetries with multiple high-order axes, classes of symmetry operations, a systematic procedure for symmetry classification of molecules. Representations of Groups: Comments on matrices and vectors, representation of groups, the "Great Orthogonality Theorem" and its consequences, character tables, representation for cyclic groups. Group Theory and Quantum Mechanics: Wave function as bases for irreducible representations, the direct product, and detection of non-zero integrals. Symmetry Adapted Linear Combinations: Derivation of Projection Operators. Use of projection operators to construct SALCs. Molecular Orbital Theory and its Application in Organic Chemistry: General remarks, Symmetry factoring of secular equations, Carbocyclic system. More general cases of LCAO-MO " bonding, naphthalene. Electronic excitations of naphthalene:

Selection rules, configuration interaction, and three-center bonding. Symmetry-based selection rules for cyclization reactions. Molecular Orbital Theory for inorganic and organometallic compounds: Transformation properties of atomic orbitals. Molecular orbitals for (J bonding in AB_n molecules: The Tetrahedral AB₄ cases. Molecular orbitals for σ bonding in AB_n molecules.

Texts book:

1. F. A. Cotton, Chemical Applications of Group Theory, 3rd Ed., John Wiley & Sons, 1990.

Reference:

1. F. L. Pilar, Elementary Quantum Chemistry, 2nd Ed., Dover Publications, INC, 1990.

CH7154

Computational Methods in Chemistry

2-0-2 6

Prerequisites: Nil

Introduction to the Linux operating system. Introduction to Fortran; Development of small computer codes involving simple formulae in chemistry: such as van der Waals equation, pH titration, kinetics, radioactive decay; Basic numerical analysis: Roots of equations, Interpolation and polynomial approximation, Numerical solution of differential equations: ODE and PDE, numerical integration, solution of linear systems using Gaussian elimination; Use of standard available software to perform simple quantum chemical calculations.

Textbooks:

1. S. J. Chapman, Fortran 90/95 for Scientists and Engineers, 2nd edition, McGraw-Hill, 2003.
2. W. E. Mayo and M. Cwiakala, Programming with FORTRAN 77, Schaum's Outline Series, McGraw-Hill, 1995.
3. Numerical Recipes in FORTRAN/C by W. H. Press, S. A. Teukolsky, W. T. Vetterling and B. P. Flannery, Cambridge University Press, 2nd edition, 1996.
4. S. C. Chapra and P. Canale, Numerical Methods for Engineers, 41h edition, Tata McGraw - Hill, 2002.
5. F. Jensen, Introduction to Computational Chemistry, 3rd edition, Wiley, 2017.

References:

1. V. Rajaraman, Computer Programming in Fortran 90 and 95, PHI, 1997.
2. M. Metcalf and J. Reid, Fortran 90/95 Explained, Oxford: O. U. P, 1999.
3. C. Xavier, Fortran 77 and Numerical Methods, Wiley Eastern, 1994.
4. J. Leszczynski (editor), Handbook of Computational Chemistry, 2nd edition, Springer, 2017.

CH7155:

Chemistry of Biological Macromolecules

3 -0 -0 6

Pre-requisites: Nil

Definition and history of chemical biology; amino acids, peptides and proteins, bio-and chemical synthesis of proteins, solid phase peptide synthesis, native chemical ligation, strategies of combinatorial synthesis, combinatorial solid phase synthesis of peptide antibiotics, post-translational modification -glycosylation, carbohydrates, oligosaccharides; lipids -fatty acids, bilayer, lipidation of proteins and peptides, farnesylation of the ras protein; biological

membranes, transport across membranes, model membrane, insertion of lipidated peptides into model membrane and their biophysical properties, concepts of fluorescence and fluorescence markers, synthesis of vesicles containing fluorescence quencher and lipidated peptides; nucleic acids -DNA double helices, DNA replication, genetic information storage, transmission and gene expression, chemical synthesis of oligonucleotides, hybridization with synthetic oligonucleotides, nucleic acids as molecular probes, peptide nucleic acids (PNAs) -synthesis, doubly labeled PNAs as probes for the detection of point mutations; use of small molecules to link a protein target to a cellular phenotype and as probes for biological processes.

Textbooks:

1. C.M. Dobson, JA Gerrard and A. J. Pratt, Foundations of Chemical Biology, Oxford Univ. Press. 2002.
2. J. M. Berg, J. L. Tymoczko and L. Stryer. Biochemistry, W. H. Freeman and Company, New York.
3. Lehninger, Nelson and Cox, Principles of Biochemistry, CBS Publishers, 1993.

References:

1. S.L. Schreiber, T. Kapoor and G. W. Wiley Chemical Biology: from small molecules to systems biology and drug design, Vol. 1, VCH Verlag GmbH & Co. 2007.
2. B. Larijani, C. A. Rosser and R. Woscholski Chemical Biology: Application and Techniques, John Wiley & Sons Ltd. England, 2006.
3. H. Waldmann and P. Janning. Wiley Chemical Biology: A practical course, VCH Verlag GmbH & Co., 2004.
4. C.M. Dobson, JA Gerrard and A.J. Pratt. Foundations of Chemical Biology, Oxford University Press, 2002.
5. A. Miller and J. Tanner, Essentials of Chemical Biology, Wiley & Sons Ltd., 2008.

CH7156P: Scientific Writing and Presentations

3-0-0-6

Prerequisites: Nil

Introduction: Research – What is it? How do researchers communicate? Types of scientific communication, Examining examples of different types of scientific communication; Scientific Literature: Searching the scientific literature, Using online search engines, What is a refereed journal? Plagiarism and how to avoid it; Beginning to Write: Establishing your constraints, Organizing your writing, Preparing outlines, Standard formats for scientific papers, research projects and theses, Style guides; Content: Creating a literature review, Preparing other sections of a research report (abstract, introduction, materials and methods, results and discussion, conclusions), Including and summarizing research data; Style and grammar: Scientific writing style, First-person vs. Third-person; Passive vs. active voice, Avoiding excessive wording, Grammar, Avoiding misuse of words, When to use footnotes; Reference citations: How to use references - Within the text, How to make lists of references; Revising: Dealing with revisions, Accepting criticism, Making sense of reviewers' comments, Making the changes, What to do if you do not agree with reviewers' comments; Other communication: Other types of scientific writing - research proposals, - creating a fact sheet/bulletin, - articles for popular press, - memos, letters and emails; Poster Presentations: Organization and formats for posters, Using Microsoft PowerPoint; Oral Presentations: Designing and preparing slides for an oral presentation,

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