

Syllabus for MSc Courses

Department of Chemistry, Indian Institute of Technology Guwahati

Semester -1

CH 4151:

Chemistry of p-and d-Block Elements

3-1-0-8

p-Block elements: Synthesis, properties, structure and bonding of nitrogen, phosphorus, sulfur, pseudohalogen, interhalogen and xenon compounds. Boranes, carboranes, metallocarboranes, borazines, phosphazenes, sulfur-nitrogen compounds, silicates, silicones, iso- and hetero-poly anions, redox reactions, Latimer diagram, electrochemical series and HSAB concept. d-Block elements: Coordination compounds-bonding in coordination complexes, crystal field theory, d-orbital splitting in octahedral, tetrahedral and square planar geometries, molecular orbital theory, pi-bonding, Jahn-Teller effect, spectrochemical series, nephelauxetic series, electronic spectra, d-d transitions, Orgel and Tanabe-Sugano diagrams, charge-transfer transitions and magnetic properties of transition metal complexes.

Textbooks:

1. J. E. Huheey, E. A. Keiter and R. L. Keiter, *Inorganic Chemistry, Principle, structure and reactivity*, 4th Ed., Harper Collins. 1993.
2. B. E. Douglas, D. H. McDaniel and J. J. Alexander, *Concepts and Models of Inorganic Chemistry*, 3rd Ed, John Wiley, 1993.
3. D. F. Shriver and P. W. Atkins, *Inorganic Chemistry*, 3rd Ed., Oxford.

References:

1. S. F. A. Kettle, *Physical Inorganic Chemistry, A Coordination Chemistry Approach*, Spektrum, 1996.
2. N. N. Greenwood and A. Earnshaw, *Chemistry of the Elements*, Pergamon, 1985.
3. F. A. Cotton, G. W. Wilkinson, *Advanced Inorganic Chemistry*, 5th Ed., John-Wiley & Sons, 1988.
4. R. S. Drago, *Physical Methods in Chemistry*, Saunders College Publishing, 1992.
5. A. B. P. Lever. *Inorganic Electronic Spectroscopy*, 2nd Ed., Elsevier, 1984.
6. A. Ernshaw, *Introduction to Magnetochemistry*, Academic Press, 1968.

Stereochemistry: Basic introduction to stereochemistry, optical activity in the absence of chiral carbon, atropisomers, spirocyclic compounds, allene systems and topicity; conformational analysis and reactivity of cycloalkane derivatives (cycloalkanes, cycloalkenes, cycloalkanones, epoxides, enones etc), medium and fused ring systems; stereoselective and stereospecific reactions-formation and reactions of enamines (proline, RAMP, SAMP) and enolates, effect of base, additives, solvents, temperature on enolate formation; asymmetric synthesis: types of asymmetric reactions, chiral auxiliaries, methods of asymmetric induction, substrate, reagent and catalyst controlled reactions; oxidation: different oxidative processes using metal- and non-metal-based oxidizing agents; hydroxylation and dihydroxylation reactions; reduction: different reductive processes including boron, aluminium, silicon, tin hydrides, dissolved metal reductions, hydrogenolysis, transfer hydrogenation, metal hydride reduction of α and β -chiral carbonyl compounds (emphasis on Cram's and Felkin-Ahn models); rearrangements: nature of migration, migratory aptitude, nucleophilic, electrophilic and free radical rearrangement reactions.

Textbooks:

1. M. B. Smith and J. March, *March's Advanced Organic Chemistry, Reactions, Mechanism and Structure*, 6th Ed., John Wiley & Sons, 2007.
2. E. J. Eliel, *Stereochemistry of Carbon Compounds*, McGraw-Hill.
3. F. A. Carey and R. J. Sundberg, *Advanced Organic Chemistry Part: A and B*, 5th Ed., Springer, 2008.
4. Peter Sykes, *A Guidebook to Mechanism in Organic Chemistry*, Pearson Education India, 1986.

Reference:

1. D. Nasipuri, *Stereochemistry of Organic Compounds: Principles and Applications*.
2. S. H. Pine, *Organic Chemistry*, McGraw-Hill, 1987.
3. J. Clayden, N. Greeves, and S. Warren, *Organic Chemistry*, 2nd Ed, Oxford University Press, 2012.
4. J. March, *Advanced Organic Chemistry*, John Wiley & Sons, 1992.
5. T.W Greene, *Protective Groups in Organic Synthesis*, Wiley-VCH, 1999.

Review of essential mathematical concepts; origin of the quantum theory, postulates of quantum mechanics, Schrödinger equation and its application on some model systems viz., free-particle and particle in a box, tunneling, the harmonic oscillator, the rigid rotator, and the hydrogen atom; the variation theorem, linear variation principle, perturbation theory, applications of variational methods and perturbation theory to the helium atom; ordinary angular momentum, generalized angular momentum, eigen functions, and eigen values of angular momentum operator, Ladder operator, addition of angular momentum, spin, antisymmetry, Pauli exclusion principle, Slater determinant wave functions; term symbol (RS and jj coupling) and spectroscopic states, term separation energies of p and d configurations, magnetic effects -spin-orbit coupling and Zeeman splitting; virial theorem, Born-Oppenheimer approximation, VB and MO theory, H_2^+ , H_2 molecule problem, Hückel molecular orbital theory and its application to ethylene, butadiene and benzene, hybridization and valence MOs of H_2O , NH_3 and CH_4 , introduction to the SCF.

Textbooks:

1. F. L. Pilar, *Elementary Quantum Chemistry*, 2nd Ed., Dover Publications, Inc. NY, 1990.

2. I. N. Levine, *Quantum Chemistry*, 7th Ed., Pearson Education India, 2016.

References:

1. P. W. Atkins and R. S. Friedman, *Molecular Quantum Mechanics*, 4th Ed., Oxford Univ. Press, 2005.

CH4154:

Group Theory and Spectroscopy

3-1-0-8

Group Theory: Definition of group, symmetry, point groups, representation of group, orthogonality theorem, irreducible representation, character table, direct sum, direct product, spectral transition probabilities and symmetry-adapted linear combinations. Spectroscopy: Electromagnetic radiation and its interaction with matter, natural line width, spectral intensity-transition probability, Maxwell-Boltzman distribution, Beer-Lambert law; microwave spectroscopy -classification of molecules, rigid and non-rigid rotator, spectral intensity, effect of isotopic substitution, Stark effect; Infrared spectroscopy -vibrational energy of diatomic molecules, harmonic oscillator, selection rules, anharmonicity, rotational-vibration spectroscopy, breakdown of Born-Oppenheimer approximation, vibration of polyatomic molecules -normal mode of vibration, group frequencies, overtone, hot bands; Raman spectroscopy -classical and quantum theories of Raman effect, pure rotational and vibrational Raman spectra, mutual exclusion principle, rotational fine structure, structural determination from Raman and infrared spectroscopy; electronic spectroscopy of molecules -energy levels, MO, vibronic transitions- Franck-Condon principle, Fortrat diagram, electronic spectra of polyatomic molecules, emission spectra, radiative and non-radiative decay Perrin's Jablonski diagram; photoelectron spectroscopy.

Textbooks:

1. FA Cotton, *Chemical Applications of Group Theory*, 3rd Ed., Wiley Interscience, 1990.
2. C. N. Banwell and E. M. McCash, *Fundamentals of Molecular Spectroscopy*, 4th Ed., Tata McGraw-Hill, 1994.
3. B. Valeur and M. N. Berberan-Santos, *Molecular Fluorescence Principles and Applications*, 2nd Ed., Wiley-VCH, 2013.

Reference:

1. G. M. Barrow, *Introduction to Molecular Spectroscopy*, McGraw-Hill.
2. N. J. Turro, *Modern Molecular Photochemistry*, University Science Books, 1991.

Experiments based on conductometry (determination of critical micellar concentration, ionic mobility, reaction kinetics, and ion-crowding effect); spectroscopy (fluorescence quenching, determination of formula of complexes and metal concentration, pK_a of indicator, etc.); chemical kinetics (determination of activation energy, enzymatic reaction and simulation studies etc.); nanomaterials (synthesis, application in sensing); spin coating; molecular modelling, surface chemistry (adsorption isotherms, contact angle measurement); study of polymorphism; polymerization (methyl methacrylate).

Textbooks:

1. B. Viswanathan, P. S. Raghavan, *Practical Physical Chemistry*, Viva Books, 2004.
2. F. A Settle, *A Handbook of Instrumental techniques for analytical chemistry*, Prentice Hall PTR, 1997.
3. R. D. Braun, *Introduction to Instrumental Analysis* Int. Ed, McGraw-Hill, 1987.

References:

1. B. Valuer, *Molecular Fluorescence Principles and Applications*, Springer, 2001.

Semester-2

Introduction to Fortran, development of small computer codes involving simple formulae in chemistry, 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 POE, numerical integration, solution of linear systems using Gaussian elimination; Use of commercial software to perform simple quantum chemical calculations.

Textbooks:

1. S. J. Chapman, *Fortran 90/95 for Scientists and Engineers*, 2nd Ed., McGraw-Hill, 2003.
2. W. E. Mayo and M. Cwiakala, *Programming with FORTRAN 77*, Schaum's Outline Series, McGraw-Hill, 1995.
4. S. C. Chapra and P. Canale, *Numerical Methods for Engineers* 4th Ed., Tata McGraw-Hill, 2002.

References:

1. W. H. Press, S. A. Teukolsky, W. T. Vetterling and B. P. Flannery, *Numerical Recipes in FORTRAN/C*, 2nd Ed., Cambridge University Press, 1996.

Reaction Mechanism: Substitution in octahedral and square planar complexes, lability, trans-effect, conjugate base mechanism, racemization, electron transfer reactions -inner sphere and outer sphere mechanism, Marcus theory. Inorganic photochemistry: Photo-substitution and photo-redox reactions of chromium, cobalt and ruthenium compounds, Adamson's rules. Lanthanides and Actinides: Spectral and magnetic properties, NMR shift reagents. Organometallic Chemistry: 18-electron rule, metal carbonyls, nitrosyls, carbonyl hydrides, isolobal analogy, dioxygen and dinitrogen compounds, metal alkyls, carbenes, carbynes, alkenes, alkynes, and allyl complexes, hydrides, metallocenes, metal arene complexes, carbonylate anions, agostic interaction, oxidative addition and reductive

elimination, insertion and elimination reactions, fluxional molecules, homogeneous and heterogeneous catalysis, metal-metal bonding and metal clusters.

Text1 books:

1. J. E. Huheey, E. A. Keiter and R. L. Keiter, *Inorganic Chemistry, Principle, structure and reactivity*, 4th Ed., Harper Collins, 1993.
2. B. E. Douglas, D. H. McDaniel and J. J. Alexander, *Concepts and Models of Inorganic Chemistry*, 3rd Ed., John Wiley, 1993.

References:

1. R. R. Jordan *Reaction Mechanism in Inorganic Chemistry*, 2nd Ed., Oxford Univ. Press, 1998.
2. F. A. Cotton and G. W. Wilkinson, *Advanced Inorganic Chemistry*, 5th Ed., John Wiley & Sons, 1988.
3. Ch. Elschenbroich, A. Salzer *Organometallics*, VCH, 2nd Ed., 1995.
4. A. Yamamoto, *Organotransition Metal Chemistry: Fundamental Concepts and Applications*, John Wiley 1986.
5. R. H. Crabtree, *Organometallic Chemistry of the Transition Metals*, 2nd Ed., John Wiley, 1993.
6. D. F. Shriver and P. W. Atkins, *Inorganic Chemistry*, 3rd Ed, Oxford, 2008.

CH 4053:

Organic Reactions Mechanisms

3-1-0-8

Classification of organic reactions: electrophilic, nucleophilic and radical substitution (aliphatic and aromatic) and elimination reactions; IUPAC system for symbolic presentation of reaction mechanisms; nucleophilic substitution at an allylic, vinylic carbon and aliphatic diagonal-, trigonal-, tetrahedral carbon, Baldwin rule of ring closure; reactive intermediates: generation, structure, stability and reactivity of carbocations, carbanions, free radicals, carbenes and nitrenes; classical and non-classical carbocations, phenonium ions, norbornyl system, neighbouring group assistance, reactivity at a bridgehead position; reactivity: thermodynamic and kinetic requirements, Hammond postulate, Curtin-Hammett principle, transition states and intermediates; methods of determining reaction mechanisms-kinetic isotopic effects; Hammett and Taft equation; addition to carbon-carbon multiple bonds: mechanistic and stereochemical aspects-addition reactions involving electrophiles, nucleophiles and free radicals, regioselectivity and chemoselectivity, orientation and reactivity; addition to cyclopropane ring; addition to carbon-hetero multiple bonds: addition of Grignard reagents, organozinc and organolithium, organocuprate reagents to carbonyl and unsaturated carbonyl compounds and to α,β -chiral carbonyl compounds; reagents in organic synthesis: use of phosphorous-, sulphur- and silicon-based reagents in organic synthesis, functional group transformations; use of dicyclohexylcarbodiimide (DCC), trimethylsilyl iodide (TMSI).

Textbooks:

1. P. Sykes, *A Guidebook to Mechanism in Organic Chemistry*, Pearson Education India, 1986.
2. Smith, M. B. and March, J. *March's Advanced Organic Chemistry, Reactions, Mechanism and Structure*, Sixth Ed., John Wiley & Sons, 2007.
3. J. Clayden, N. Greeves, and S. Warren, *Organic Chemistry*, 2nd Edition, Oxford University Press, 2012.
4. P.S. Kalsi, *Organic Reaction and their Mechanism*, New Age, 1996.
5. Francis A. Carey, Richard J. Sundberg, *Advanced Organic Chemistry: Part A: Structure and Mechanisms*, 5th Ed., Springer, 2008.

Reference:

1. A. Jacobs, *Understanding Organic Reaction Mechanism*, Cambridge 1998.
2. W. Carruther, *Some Modern Methods of Organic Synthesis*, Cambridge, 1990.
3. J. M. Hornback, *Organic Chemistry Books*, Coley, 1998.

4. P. Y. Bruice, *Organic Chemistry*, Prentice Hall, 1998.
5. S. H. Pine, *Organic Chemistry*, McGraw-Hill, 1987.
6. R. O. C. Norman and J. M. Coxon, *Principle of Organic Synthesis*, CRC Press , 1993.

CH 4054L: Organic Chemistry Laboratory

0-0-9-9

Separation techniques and characterization (TLC, column chromatography, distillation, crystallization, GC etc.). Organic synthesis: Representative reaction of esterification and saponification, oxidation, reduction, nucleophilic substitution, cycloaddition reactions, Grignard reaction, Suzuki coupling, condensation reactions, preparation of dyes, aromatic electrophilic substitution, heterocyclic synthesis, solid phase synthesis, natural product extraction -solasidine, caffeine, nicotine, peptine, rosine and carotenoids.

Textbooks:

1. B. S. Furniss, *Vogel's Text Book of Practical Organic Chemistry*, 5th Ed., ELBS Longman, 1996.
2. A. Ault, *Techniques and Experiments for Organic Chemistry*, 6th Ed., University Science Book, 1998,
3. F. Settle, *Instrumental techniques for Analytical Chemistry*, Printice Hall, 1997.

CH 4055: Chemical Dynamics and Electrochemistry

3-1-0-8

Chemical Dynamics: Collision theory of reaction rates, Arrhenius equation, activated complex theory, kinetic and thermodynamic control of reactions, ionic reactions, kinetic salt effects, unimolecular reactions and their treatments (Lindemann-Hinshelwood and Rice-Ramsperger-Kassel-Marcus [RRKM] theory), complex reactions (chain reactions, and oscillatory reactions), photochemical reactions, homogeneous catalysis, enzyme kinetics, studies of fast reactions by flow method, relaxation method; dynamics of molecular reactions, probing the transition state, dynamics of barrierless chemical reactions in solution, dynamics of unimolecular reactions. Electrochemistry: Electrochemical cells, Nernst equation, applications of Debye-Hückel theory, electrolytic conductivity and the Debye-Hückel-Onsanger treatment, electrified interfaces -overpotential, corrosion.

Textbooks:

1. K. Laidler, *Chemical Kinetics*, Harper and Row, 1995.
2. K. A. Connors, *Chemical Kinetics: The study of reaction rates in solution*, VCH , 1990.
3. C. H. Hamann, A. Hamnett and W. Vielstich, *Electrochemistry*, 2nd Ed., Wiley VCH, 2007,

References:

1. M. J. Pilling and P. W. Seakins, *Reaction Kinetics*, Oxford Press, 1997,
2. J. O. Bockris and A. K. N. Reddy, *Modem Electrochemistry 1*, Volume 1 and 2, Kluwer Academic, 2000.

CH 4056: Applications of Spectroscopy

3-1-0-8

Inorganic spectroscopy: vibrational -symmetry and shapes of AB₂ AB₃ AB₄, AB₅ and AB₆, modes of bonding in ambidentate ligands; electron spin resonance -hyperfine coupling, spin polarization, spin-orbit coupling and g-tensor, application to transition metal complexes with one unpaired electron, inorganic and organic free radicals; Mossbauer basic principles -Mossbauer effect, isomer shift, electric quadrupole splitting, hyperfine magnetic field splitting, examples of spectra, valence and spin determination of Mossbauer active nuclei including ⁵⁷Fe and ¹¹⁹Sn, Organic spectroscopy:

Woodward rule, characteristic vibrational frequencies of different functional groups, effect of hydrogen bonding and solvent effect on vibrational frequencies; Nuclear Magnetic Resonance: nuclear relaxation, chemical shift, spin-spin interaction, shielding, virtual coupling hindered rotation, Karplus curve, nuclear magnetic double resonance, simplification of complex spectra, shift reagent, spin tickling, nuclear Overhauser effect (NOE), resonance of other nuclei, ^{13}C NMR - chemical shift and coupling constants, two-dimensional NMR spectroscopy. Mass spectrometry: Instrumentation, mass spectral fragmentation of organic compounds, McLafferty rearrangement. Structure determination using different techniques.

Textbooks:

1. R. S. Drago, Physical Methods in Chemistry, Saunders, 1992.
2. A. B. P. Lever, Inorganic Electronic Spectroscopy, 2nd Ed., Elsevier, 1984.
3. R. M. Silverstein, Spectrometric Identifications of Organic Compounds, John Wiley, 1991.
4. D.L. Pavia, G. M. Lampman, G. S. Kriz, Introduction to Spectroscopy, Harcourt College Publishers, NY, 2001.

References:

1. W. Kemp, Organic Spectroscopy, 3rd Ed., ELBS, 1994.

Semester-3

CH 5151:

Principles of Bioinorganic Chemistry

3-1-0-8

Role of alkali and alkaline earth metal ions in biology, Na^+ - K^+ pump, ionophores and crown ethers. Metal site structure and function: metal ion transport and storage -ferritin, transferrin, siderophores and metallothionein; electron transfer -cytochromes, iron-sulfur proteins and copper proteins; oxygen transport and storage -hemoglobin, myoglobin, hemerythrin, hemocyanin; oxygen activation cytochrome P450, cytochrome c oxidase; other metal containing enzymes -catalase, peroxidase, superoxide dismutase, alcohol dehydrogenase, carbonic anhydrase, carboxypeptidase, xanthine oxidase, nitrogenase, vitamin B12coenzyme, photosystem I and II, oxygen evolving center. Use of coordination complexes as models for various enzymes, metalloproteins, role/effect of species such as nitric oxide, cyanide, methyl isocyanate, etc., in biological systems. Applications of electronic, EPR (3d metals only), resonance Raman, multinuclear NMR, CD/MCD, EXAFS, XANES and ENDOR techniques in bioinorganic chemistry.

Textbooks:

1. S. J. Lippard and J. M. Berg, Principles of Bioinorganic Chemistry, University Science Books, 1994.
2. L. Que Jr, Physical Methods in Bioinorganic Chemistry: Spectroscopy and Magnetism, University Science Books, 2000.

References:

1. F. A. Cotton and G. W. Wilkinson, Advanced Inorganic Chemistry, 5th Ed., John-Wiley & Sons, 1988.
2. D. Banerjee, Coordination Chemistry, 2nd Ed., Asian Books Pvt. Ltd., 2007.
3. J. E. Huheey, E. A. Keiter and R. L. Keiter, Inorganic Chemistry, Principle, structure and reactivity, 4th Ed., Harper Collins, 1993.

Pericyclic Reactions: symmetry of molecular orbitals, frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl system, classification of pericyclic reactions; Woodward-Hoffmann correlation diagrams, FMO and PMO approaches; electrocyclic reaction -conrotatory and disrotatory motions of $4n$, $4n+2$ and allyl systems; cycloaddition -antarafacial and suprafacial addition, $4n$ and $4n+2$ systems, $2+2$ addition of ketenes, 1,3 dipolar cycloadditions and cheletropic reactions; sigmatropic rearrangements -suprafacial and antarafacial shifts of hydrogen, sigmatropic shifts involving carbon moieties, 3,3-and 5,5-sigmatropic rearrangements, Claisen, Cope and Aza-Cope rearrangements, ene reaction. Photochemistry: quantum yields, photosensitization and energy transfer reactions, photochemistry of olefins and carbonyl compounds, photo oxygenation and photo fragmentation, photochemistry of aromatic compounds -isomerization, additions and substitutions, singlet oxygen reactions, Paterno-Buchi reaction, di- π -methane rearrangement, Barton reaction, Photo-Fries rearrangement. transition-metal catalyzed reactions: Suzuki, Heck, Stille, Kumada, Negishi, Buchwald-Hartwig amination and Sonogashira couplings, Grubb's catalyst, Peterson's synthesis, Wilkinson's catalyst, Merrifield resin and Baker's yeast. Heterocyclic Chemistry: Synthesis and reactivity of furan, thiophene, pyrrole, pyridine, quinoline, isoquinoline and indole and related name reactions. Chemistry of natural products: basic introduction and classification of natural products-alkaloids, terpenoids and steroids.

Textbooks:

1. I. Fleming, Frontier Orbital and Organic Chemical Reactions, Wiley, 1976.
2. J. Singh and J. Singh, Photochemistry and Pericyclic Reactions, New Age Int. Publishers. Ltd., New Delhi, Ed. 3rd, 2010.
3. J. A. Joule, K. Mills, Heterocyclic Chemistry, 5th Ed., Wiley-Blackwell, 2010.
4. W. Carruthers, Some Modern Methods of Organic Synthesis, Cambridge University Press, 1990.
5. I. L. Finar, Organic Chemistry, Vol II, ELBS, 1968.

Reference:

1. L. A. Paquette, Modern Heterocyclic Chemistry, WA Benjamin Inc, 1968.
2. T. R. Gilchrist, Longman, Heterocyclic Chemistry, 1989.
3. Ward, Selectivity in Organic Synthesis, Wiley-VCH, 1999.
4. M. J. S. Dewar and R. C. Dougherty, The PMO Theory of Organic Chemistry, Springer-Verlag New York Inc., 2011.

Overview of bioorganic chemistry, historical connection between organic and biological chemistry, weak interactions in organic and biomolecules, chemistry of the living cells; analogy between biochemical and organic reaction; basics of proteins-structures, properties and sequencing; introduction to enzyme catalysis and kinetics, enzyme inhibition and drug design, enzymes in organic synthesis; antibody catalyzed organic reactions; basics of nucleic acids-structures and functions of DNA and RNA, DNA mutations, sequencing of DNA, chemical synthesis of nucleic acids; biosynthesis of proteins; biomimetic chemistry; expanding the genetic alphabets and genetic code -background and applications; drug-DNA interactions, catalytic RNA, siRNA, micro RNA; Carbohydrates: structure and conformations; glycoproteins, role of sugars in biological recognition; lipids and membranes: Common classes of lipids, self-association of lipids, liposomes, biological membranes and models.

Textbooks:

1. H. Dugas, Bioorganic Chemistry-A Chemical Approach to Enzyme Action, 3rd Ed., 1996.
2. C. Schmuck (Editor), H. Wennemers (Editor), R. Breslow (Foreword by), Highlights in Bioorganic Chemistry: Methods and Applications, Wiley, 2004.
3. G. Ebert, Biomimetic and Bioorganic Chemistry, Springer Verlag, 1985
4. Nelson and Cox, Lehninger Principles of Biochemistry, 61h Ed., 2013.

References:

1. U. Diederichsen (Editor), T. K. Lindhorst (Editor), B. Westermann (Editor), L. A. Wessjohann (Editor), Bioorganic Chemistry: Highlights and New Aspects, Wiley, 1999.
2. S. S. Bag, NPTEL-Web-based Course, Bio-Organic Chemistry. Website: <https://nptel.ac.in/courses/104103018>
3. A. Miller and J. Tanner, Essentials of Chemical Biology, Wiley & Sons Ltd., 2008.
4. R. B. Silverman, The organic chemistry of enzyme-catalyzed reactions, 717 pp, Academic Press, San Diego, 2000.

CH 5154:

Classical and Statistical Thermodynamics

3-1-0-8

Classical thermodynamics: Review of the laws of thermodynamics, free energy, chemical potential and entropies; partial molar quantities and their significances; determination of these quantities, concept and determination of fugacity; non-ideal systems: excess function for non-ideal solutions; application of phase rule to three-component systems; second-order phase transitions. Statistical thermodynamics: Statistical concepts and examples, simple random walk problem in one dimension; general discussion of mean values and its use for the random walk problem; specification of the state; statistical ensembles; basic postulates; probability calculations; behavior of the density of states; exact and inexact differentials; equilibrium conditions and constraints; reversible and irreversible processes; distribution of energy between systems in equilibrium; isolated system; system in contact with heat reservoir; canonical distribution and its simple applications; ensembles used as approximation; calculation of thermodynamic quantities, Gibbs paradox, validity of the classical approximation, equipartition theorem and its applications -specific heats of solids, Maxwell velocity distribution; quantum statistics of ideal gases; identical particles and symmetry requirements; quantum distribution functions; Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac statistics; quantum statistics in the classical limit; electromagnetic radiation in thermal equilibrium inside an enclosure; consequences of Fermi-Dirac equation; Lattice vibration and normal modes; Debye approximation.

Textbooks:

1. R. S. Berry, S. A. Rice and J. Ross, Physical Chemistry, 2nd Ed., Oxford University Press, 2000.
2. F. Reif, Fundamentals of Statistical and Thermal Physics, McGraw-Hill, International, 1985.

Reference:

1. D. A. McQuarrie and J. D. Simon, Physical Chemistry: A Molecular Approach, 3rd Ed., University Science Books, 2001.
2. R. K. Pathria Butterworth-Heinemann, Statistical Mechanics, 2nd Ed. 1999.
3. B. Widom, Statistical Mechanics, Cambridge University Press, 2002.

CH5155L:

Inorganic Chemistry Laboratory

0-0-9-9

Synthesis and characterization of inorganic compounds, including coordination complexes and assemblies. Synthetic methods: solution chemistry, solid state synthesis, sol-gel methods, multistep synthesis, preparation of isomers, synthesis under inert atmosphere, and electrosynthesis. Characterization: quantitative and qualitative determination of ligand and metal, use of spectral techniques (UV -visible, IR, NMR, ESR, magnetic moment, analytical methods -conductance, TG, DSC, cyclic voltametry, coulometry).

Textbooks:

1. G. S. Girolami, T. B. Rauchfuss and R. J. Angelici, Synthesis and Technique in Inorganic Chemistry: A Laboratory Manual, University Science Books.
2. W. A. Herrmann, G. T. Verlag, Synthetic methods of organometallic and inorganic chemistry, Vol 7 and 8, New York, 1997.
3. G. Svehla, Vogel's qualitative inorganic analysis, Harlow: Longman, 1996.
4. A. I. Vogel, Vogel's textbook of quantitative inorganic analysis: including elementary instrumental analysis 4th Ed., John Bassett et al., London; New York: Longman, 1978.

Semester-4

CH5051P:

Graduate Seminar

0-0-2-2

In this course, students will be taught how to give a PowerPoint presentation using selected articles from internationally reputed journals covering research in Inorganic, Organic, and Physical Chemistry. Preliminary idea may also be given on how to write a scientific article or part of it.

CH5052P:

Project

0-0-18-18

Elective Courses

CH5053:

Inorganic Clusters

(3-0-0-6)

Metal bonding: metal-metal multiple bonds, bonding in dinuclear metal compounds, bonding multiplicity and internal rotation, compounds with bond order four, three, and two. Transition metal clusters: classification, structural characteristics, cluster geometries, trinuclear, tetra nuclear, pentanuclear, hexanuclear metal clusters, bonding in metal clusters, polyhedral skeletal electron pair theory, isolobal relationships, platinum and gold clusters, synthesis of cluster compounds, cluster reactivity, catalysis by metal clusters. Cluster species of alkali metals. Main group-transition metal mixed clusters: structure and bonding in hydride cluster compounds, carbido-clusters. Main group elements: clusters and cages, boron hydrides and carboranes, phosphorus cage compounds. Posttransition elements: zintl anions.

Textbooks:

1. Cluster Chemistry by G. G. Moraga, Springer-Verlag, 1993.
2. Molecular clusters: a bridge to solid-state chemistry by T.P. Fehlner, J. Halet, J. Saillard, Cambridge University Press, 2007.

References:

1. Multiple Bonds Between Metal Atoms by F. A. Cotton, C. A. Murillo and R. A. Walton, (Eds.) Springer Science and Business Media, Inc. 2005
2. Molecular Clusters of the Main Group Elements by M. Driess, H. Noth (Eds.) Wiley-VCH, 2004.

CH5054:

Applied Inorganic Chemistry

(3-0-0-6)

Pre-requisites: Basic knowledge in inorganic chemistry and organometallic chemistry.

Catalysis: Homogeneous & heterogeneous catalysis, C-C bond formation, C-H activation, RCM. Medicinal: MRI contrast agents, anticancer metallodrugs and related compounds. Inorganic Polymer: Polyoxometalates and their applications, MOFs and their application. Non-conventional sources of energy: Photochemical methods, transition-metal complexes for energy production, catalytic CO₂ reduction, solar hydrogen system. Nano-materials: Definition of nano-materials, properties and applications of nano-materials. Sensor: Anionic sensors, cationic sensors, pesticide sensors, and explosive sensors.

Textbooks:

1. Inorganic Chemistry: Principles of Structure and Reactivity by J. E. Huheey, E. A. Keiter and R. L. Keiter, 4th Ed. Harper Collins, 1993.
2. Organotransition metal chemistry, Fundamental concept and applications, A. Yamamoto, John Wiley, 1986.
3. Gd-containing nanoparticles as MRI contrast agents, Nicolaij, K, Klaas, Strijkers, GJ Gustav Gröll, H Holger, Wiley, 2013.
4. Coordination Polymers and Metal Organic Frameworks: Properties, Types, and Applications, Ortiz, scar L., 2011.

References:

1. Chemical sensor fundamentals of sensing materials 1st Ed. by Ghenadii Korotcenkov. -New York: Momentum Press, 2010.
2. Nano-architected and nanostructured materials: fabrication, control and propertie, 1st Ed. by Y. Champion and H. -J. Fecht-Weinheim: Wiley-VCH, 2004.
3. Organic photovoltaics mechanisms materials and devices, 1st Ed by Sam-Shajing Sun and Niyazi Serdar Saricifrci. -Boca Raton: CRC Press, 2005.
4. Catalysis by polyoxometallates/ ivan V. Kozhevnikov . -Chichester: John Wiley & Sons, 2002.
5. Advances in Anticancer Agents in Medicinal Chemistry, by Prudhomme, Michelle, 2013.

CH5055:

Supramolecular Chemistry

3 0 0 6

Host-Guest Chemistry: Definition, classifications of host-guest compounds, thermodynamics and kinetic stability, role of weak interactions in supramolecules, Complementarity and cooperativity, hydride sponge and related clathrates. Different macromolecular hosts: host design, preorganised hosts, cyclodextrins, calixarenes, cucurbiturils etc. Recognition and reactivity: molecular and Ion recognition, enantioselectivity, proton pumps and basis of supramolecular catalysis. Inorganic host design: Metal-directed assemblies, confinement, container molecules, molecular flasks, layered solids, channel structures, Intra-cavity complexes of neutral molecules. Physical methods in understanding supramolecular chemistry: Determination of binding constant, Isothermal titration calorimetry, rheology, SEM, TEM etc. Supramolecular polymers: Co-ordination polymers,

hydrogen bond-based polymers, guest-included polymers, examples and applications. Supramolecular gels: hydrogel and organogel, transient gels, and their applications. Molecular machines: Interlocked dynamic systems, molecular motors, switches, and shuttles. Amphiphiles and their self-aggregation: micelle, vesicles, liposomes, microemulsions. Host J aggregates, aggregation-induced emission and quenching. Natural processes: Peptide self-assembly, Protein and DNA aggregation, amyloid and cell membrane.

Textbooks:

1. J. W. Steed and J. L. Atwood, Supramolecular chemistry, Wiley, New York, 2000.
2. J. M. Lehn, Supramolecular Chemistry, VCH, New York, 1995.
3. H. J. Schneider and A. Yatsimirsky, Principles and methods in Supramolecular chemistry, Wiley, New York, 2000.

References:

1. J. L. Atwood, J. E. D. Davies, D. D. McNicol and F. Vogtle (Exe. Ed), Comprehensive Supramolecular Chemistry, Pergamon, New York, 1996.
2. C Schalley (Ed), Analytical Methods in Supramolecular Chemistry, Wiley-VCH.

CH5056: Modern Reagents in Organic Synthesis

3 0 0 6

Lanthanides in Organic Synthesis: General properties of Lanthanides, use of Lanthanide metal compounds at different oxidation states in synthesis. Reagents from cerium, samarium, ytterbium etc. Organotransition metal reagents: principles, reagents developed from titanium, chromium, iron, rhodium, nickel, palladium, ruthenium, molybdenum, copper, silver, gold, manganese, cobalt, zirconium, iridium etc. Synthetic applications of metal-hydride, metal-carbon σ -bonds, metal-carbonyl complex, metal-carbene complex, metal-alkene, -alkyne and -arene complexes. Advanced reagents containing phosphorus, sulfur, silicon and boron.

Texts books:

1. R. O. C. Norman and J. H. Coxon, Principle of Organic Synthesis, 1st Ed, ELBS, 1993.
2. T. Imamoto, Lanthanides in Organic synthesis, Academic Press, 1994,
3. W. Carrutier, Some Modern methods of Organic Synthesis, Cambridge, 1990,
4. L. W. Paquette (Ed), Reagents for Organic synthesis, John Wiley, 1995,
5. Andre B. Charette, Handbook of Reagents for Organic Synthesis: Reagents for Heteroarene Synthesis, Wiley-Blackwell, 1 edition, 2017.

References:

- 1, T.W. Greene, Protective Groups in Organic Synthesis Wiley-VCH, 1999.
- 2, B. P. Mundy, M. G. Ellerd, and F. G. Favalaro Jr., Name Reactions and Reagents in Organic Synthesis, Wiley, 2nd Ed. 1988.

CH5057: Advanced Quantum Chemistry

3 0 0 6

Pre-requisites: Prior knowledge of Quantum Chemistry

Introduction: Vector interpretation of wave function, Hermitian operator, approximate solutions to the Schrödinger equation: the variation method (time independent and time dependent), time

independent perturbation theory (non-degenerate and degenerate), time dependent perturbation theory; electron spin and many -electron systems: the antisymmetry principle, spin angular momenta and their operators, the orbital approximation (Slater determinant, Pauli exclusion principle), two electron wavefunctions; the Hartree-Fock selfconsistent field method: the generation of optimized orbitals, Koopman' s theorem (the physical significance of orbital energies), the electron correlation energy, density matrix analysis of the Hartree-Fock approximation, natural orbitals, the matrix solution of the Hartree-Fock equations (Roothaan's equations); introduction to molecular structure: the Born-Oppenheimer approximation, solution of the nuclear equation, molecular Hartree-Fock calculations, electronic structure of linear molecule: the MO-LCAO approximation, the hydrogen molecular ion, the hydrogen molecule, molecular configuration-interaction calculations.

Textbooks:

1. F. L. Pilar, Elementary Quantum Chemistry, 2nd Ed., Dover Publications, 1990.
2. I. N. Levine, Quantum Chemistry, 7th Ed., Pearson Education India, 2016
3. Szabo and Ostlund, Modern Quantum Chemistry, Dover Publications, Inc., NY, 1989.

References:

1. D. A. McQuarrie, Quantum Chemistry, Oxford Univ. Press, 1983.
2. P. W. Atkins and R. S. Friedman, Molecular Quantum Mechanics, 4th Ed., Oxford Univ. Press, 2005.

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Principles and Applications of Molecular Fluorescence

3-0-0-6

Pre-requisites: Nil

Absorption and emission of light, radiative and non-radiative transitions, fluorescence and phosphorescence emission, delayed fluorescence, laws of photochemistry, principles of steady-state and time resolved fluorometric techniques, time-domain and frequency-domain lifetime measurements, lifetimes and quantum yield, effects of solvents, temperature and molecular structure on fluorescence spectra, mechanisms of quenching, photoinduced electron and proton transfer, resonance energy transfer, fluorescence polarization, extrinsic causes of fluorescence depolarization, additivity law, free and hindered rotation, effect of rotational diffusion on fluorescence anisotropies: the Perrin equation, molecular probes and sensors, optical clinical chemistry and spectral observables and mechanisms of sensing.

Textbooks:

1. B. Valuer, Molecular Fluorescence, Wiley-VCH, 2002.
2. J. R. Lakowicz, Principles of Fluorescence Spectroscopy, Springer, 3rd Ed. 2006.

References:

1. J. R. Lakowicz, Topics in Fluorescence Spectroscopy, Vol. 1: Techniques, Plenum Press, 1991.
2. J. R. Lakowicz, Topics in Fluorescence Spectroscopy, Vol. 4, Probe Design and Chemical Sensing, Kluwer Academic Press, 1994.
3. B. Valuer and J. C. Brochon, New Trends in Fluorescence Spectroscopy: Applications to Chemical and Life Sciences, Springer, 2001
