Annexure-96/IPPC/6

DEPARTMENT OF CHEMISTRY

INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI

Course Structure and Syllabus for M. Sc. In Chemistry

Course No.	Course Name	L	T	P	C		Course No.	Course Name	L	T	P	C
Semester - 1							**Semester - 2**					
CH 410	Chemistry of *p*- and *d*-Block Elements	3	1	0	8		CH 400	Computers and Chemistry	2	0	2	6
CH 420	Principles of Organic Chemistry	3	1	0	8		CH 411	Inorganic Reaction Mechanism and Organometallics	3	1	0	8
CH 430	Quantum Chemistry	3	1	0	8		CH 421	Organic Reactions Mechanisms	3	1	0	8
CH 431	Group Theory and Spectroscopy	3	1	0	8		CH 425	Organic Chemistry Laboratory	0	0	9	9
CH 435	Physical Chemistry Laboratory	0	0	9	9		CH 432	Chemical Dynamics and Electrochemistry	3	1	0	8
							CH 433	Applications of Spectroscopy	3	1	0	8
		12	**4**	**9**	**41**				**14**	**4**	**11**	**47**
Semester - 3							**Semester - 4**					
CH 511	Principles of Bioinorganic Chemistry	3	1	0	8		CH 500	Graduate Seminar	0	0	2	2
CH 520	Concepts in Organic Synthesis	3	1	0	8		CH 600	Project	0	0	18	18
CH 521	Bio-organic Chemistry	3	1	0	8		CH 6XX	Elective I	3	0	0	6
CH 530	Classical and Statistical Thermodynamics	3	1	0	8		CH 6XX	Elective II	3	0	0	6
CH 515	Inorganic Chemistry Laboratory	0	0	9	9				**6**	**0**	**20**	**32**
		12	**4**	**9**	**41**		**Total**		**44**	**12**	**49**	**161**

M. Sc. Elective Courses

CH 611 Advanced Organometallic Chemistry 3 0 0 6
CH 612 Inorganic Clusters 3 0 0 6
CH 613 Applied Inorganic Chemistry 3 0 0 6
CH 621 Modern Reagents in Organic Synthesis 3 0 0 6
CH 622 Methods in Organic Synthesis 3 0 0 6
CH 623 Supramolecular Chemistry 3 0 0 6
CH 624 Fundamentals of Chemical Biology 3 0 0 6
CH 632 Solid State and Interfacial Chemistry 3 0 0 6

Common Elective Courses

CH 603 Concepts for Molecular Machine 3 0 0 6
CH 614 Supramolecules: Concepts and Applications 3 0 0 6
CH 615 Applied Crystallography 3 0 0 6
CH 625 Advances in Biological Macromolecules 3-0-0-6
CH 631 Advanced Quantum Chemistry 3 0 0 6
CH 639 Principles and Applications of Molecular Fluorescence 3 0 0 6

Semester – 1

CH 410: Chemistry of *p*- and *d*-Block Elements 3-1-0-8

p-Block elements: Synthesis, properties, structure and bonding of nitrogen, phosphorous, 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.

Text 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.
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.

CH 420: Principles of Organic Chemistry 3-1-0-8

Stereohemistry: 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 elonate 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.

Text books:

1. M. B. Smith and J. March, *March's Advanced Organic Chemistry, Reactions, Mechanism and Structure*, Sixth 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 Edition, 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.

CH 430: Quantum Chemistry 3-1-0-8

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 determinantal wave functions; term symbol (RS and jj coupling) and spectroscopic states, term separation energies of p^n and d^n 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, hybridisation and valence MOs of H_2O, NH_3 and CH_4, introduction to the SCF.

Text books:
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.

CH 431: 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, harmonicoscillator, 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.

Text books:
1. F.A. 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.

CH 435: Physical Chemistry Laboratory 0-0-9-9

Experiments based on conductometry (determination of critical micelle 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).

Text books:

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

CH 400: Computers & Chemistry 2-0-2-6

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 PDE, numerical integration, solution of linear systems using Gaussian elimination; Use of commercial software to perform simple quantum chemical calculations.

Text books:

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.

CH 411: Inorganic Reaction Mechanism and Organometallics 3-1-0-8

Reaction Mechanism: Substitution in octahedral and square planar complexes, lability, trans-effect, conjugate base mechanism, racemisation, 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, cabonyl 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.

Text 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., JohnWiley& 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., JohnWiley, 1993.
6. D. F. Shriver and P. W. Atkins, *Inorganic Chemistry*, 3rd Ed., Oxford, 2008.

CH 421: 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, regio-selectivity and chemo-selectivity, 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 and 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, trimethylsilyl iodide.

Text books:
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. Carrutuer, *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 425: 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 couling,condensation reactions, preparation of dyes, aromatic electrophilic substitution, heterocyclic synthesis, solid phase synthesis, natural product extraction - solasidine, caffeine, nicotine, peptine, rosine and carotenoids.

Text books:
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 432: 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 barrier-lesschemical reactions in solution, dynamics of unimolecular reactions. Electrochemistry: Electrochemical cells, Nernst equation, applications of Debye-Huckel-theory, electrolytic conductivity and the Debye-Hückel-Onsangar treatment, electrified interfaces -overpotential, corrosion.

Text books:
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, *Modern Electrochemistry 1*, Volume 1 and 2, Kluwer Academic, 2000.

CH 433: Applications of Spectroscopy,3-1-0-8

Inorganic spectroscopy: vibrational - symmetry and shapes of AB_2, AB_3, AB_4, AB_5 and AB_6, 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; Mössbauer basic principles – Mössbauer effect, isomer shift, electric quadrupole splitting, hyperfine magnetic field splitting, examples of spectra, valence and spin determination of Mossbauer active nuclei including ^{57}Fe and ^{119}Sn.
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.

Text books:

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 Publisher, NY, 2001.

References:

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

Semester – 3

CH 511: 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 (3*d*metals only), resonance Raman, multinuclear NMR,CD/MCD, EXAFS, XANES and ENDOR techniques in bioinorganic chemistry.

Text books:

1. S. J. Lippard and J. M. Berg, *Principle 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*, 5thEd. , John-Wiley & Sons, 1988.
2. D. Banerjea, *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.

CH 520: Concepts in Organic Synthesis 3-1-0-8

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 –antara facial and suprafacial addition, 4n and 4n+2 systems, 2+2 addition of ketenes, 1,3 dipolar cycloadditions and cheleotropic reactions; sigmatropic rearrangements - suprafacial and antarafacial shifts of hydrohen, 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 -isomerisation, additions and substitutions, singlet oxygen reactions, Patterno-Buchi reaction, di-pi-methane rearrangement, Bartons reaction, photo-Fries rearrangement. transition-metal catalyzed reactions: Suzuki, Heck, Stille, Kumada, Negishi, Buchwald-Hartwig amination and Sonogoshira 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.

Text books:

1. I. Fleming, *Frontier Orbital and Organic Chemical Reactions,* Wiley, 1976.
2. J. Singh and J. Singh, *Photochemistry and Pericyclic Reactions*, New Age Intl. 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*, W.A. 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.

CH 521: Bioorganic Chemistry 3-1-0-8

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.

Text books:

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*, 6th 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: http://www.nptel.iitm.ac.in/courses/104103018/
3. A. Miller and J. Tanner, *Essentials of Chemical Biology*, Willey & Sons Ltd., 2008.
4. R. B. Silverman, *The organic chemistry of enzyme-catalyzed reactions,* 717 pp, Academic Press, San Diego, 2000.

CH 530: 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 ofphase 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; behaviour 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-Boltzman, 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.

Text books:

1. R. S. Berry, S. A. Rice and J. Ross, *Physical Chemistry*, 2nd Ed., Oxford University Press, 2000.
2. F. Reif, *Fundamental 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.

CH 515: Inorganic Chemistry Laboratory 0-0-9-9

Synthesis and characterization of inorganic compound including coordination complexes, assemblies.Synthetic methods: solution chemistry, solid state synthesis, sol-gel methods, multistep synthesis, preparation of isomers, synthesis under inert atmosphere, 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).

Text books:

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

CH 500: Graduate Seminar 0-0-2-2

In this course the students will be taught how to give power point presentation from chosen Articles from international reputed journals covering the research on Inorganic, Organic and Physical Chemistry. Preliminary idea may also be given how to write a scientific articles or part of it.

CH 600: Project 0-0-18-18

Elective Courses

CH 611: Advanced Organometallic Chemistry 3-0-0-6

Definition, classifications and bonding in organometallic compounds; isolobalanalogies, structural methods of organometallics;preparative methods; spectroscopic techniques in organometallic chemistry; electronic and magnetic properties of organometallic compounds; stoichiometric and catalytic reactions; fundamental processes in reactions of organo-transition metal complexes, applications of transition metal complexes to catalysis, organometallics directedtowards organic synthesis, bio-organometallics, organometallics in environmental chemistry; metal clusters and models for heterogeneous catalysis;application of organometallics in industry.

Text books:

1. P. Perez, Advances in Organometallic Chemistry, Volume 65, 1st Edition, Academic Press, 2016.
2. A.Yamamoto, *Organotransition metal chemistry, Fundamental concept and applications*, John Wiley, 1986.
3. R.H. Crabtree, *The organometallic Chemistry of transition metals*, John Wiley, 1994.

References:
1. Armando J. L. Pombeiro, Advances in Organometallic Chemistry and Catalysis: The Silver/Gold Jubilee International Conference on Organometallic Chemistry Celebratory Book, John Wiley & Sons, Inc., 2013

CH 612: 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, tetranuclear, 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. Post-transition elements: zintl anions.

Text Books:
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.

CH 613: 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 CO_2 reduction, solar hydrogen system. Nano-materials: Definition of nano-materials, properties and applications of nano-materials. Sensor: Anionic sensors, cationic sensors, pesticides sensors, explosive sensors.

Text Books:
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 Grüll, 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 / ed. by Ghenadii Korotcenkov . - New York: Momentum Press, 2010.
2. Nano -architectured and nanostructured materials: fabrication, control and properties / ed. by Y. Champion and H. -J. Fecht . -Weinheim: Wiley-VCH, 2004.
3. Organic photovoltaics mechanisms materials and devices / 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.

CH 621: 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. Organo-transition 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 phosphorous, sulphur, 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, *Lanthenides in Organic synthesis*, Academic Press, 1994.
3. W. Carrutuer, *Some Modern methods of Organic Synthesis*, Cambridge, 1990.
4. L. W. Paqueette(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. Favaloro Jr., *Name Reactions and Reagents in Organic Synthesis*, Wiley, 2nd Ed. 1988.

CH 622: Methods in Organic Synthesis 3 0 0 6

Retrosynthetic Analysis: Basic for retrosynthetic analysis, transforms and retrons, types of transforms, biomimitic 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 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 and picrotoxinin.

Texts books:

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.

References:

1. G. S. Zweifel, M. H. Nantz and Peter Somfai, *Modern Organic Synthesis: An Introduction*, 2nd Ed., Wiley 2017.
2. S. Warren, P. Wyatt, *Workbook for Organic Synthesis: The Disconnection Approach*, 2nd Ed., 2010.

CH 623: 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 coperativity, hydride sponge and related clathrates. Different macromolecular hosts: host design, preorganised hosts, cyclodextrins, calixarenes, cucurbiturils etc. Recognition and reactivity: molecular and Ion recognition, enatioselectivivity, 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, switch, and shuttles. Amphiphiles and their self-aggregation: micelle, vesicles, liposomes, microemulsions. H and J aggregates, aggregation induced emission and quenching. Natural processes: Peptide self-assembly, Protein and DNA aggregation, amyloid and cell membrane.

Text books:

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.

CH 624: Fundamentals of Chemical Biology 3 0 0 6

Chemical biology: definition, history of origin; Tools and techniques of chemical biology- High-Throughput Screening, combinatorial strategies, screening of drugs; proteomics-introduction, biosynthesis of protein, structure and function of the proteins, protein sequencing, post-translational modifications; biomolecular interactions: protein-ligand, protein-protein, DNA-protein, RNA-protein, protein-carbohydrate and lipid-protein interactions; molecular sensing- native chemical ligation,chemical affinity tags, probes and assays for the characterization of complex protein samples and biomolecular interactions; glycobiology- structure, biological functions and biosynthesis of saccharides, glycomics, glycans in medicine and vaccine development, carbohydrate based vaccines-challenges and design; RNAi/miRNA pathway and its regulation, siRNA-a tool in chemical biology; small molecules as probes of proteins/enzymes;protein kinases as anticancer drug targets; manipulation of protein functions and biological activity with small molecules, proteolysis targeting chimeric molecules (PROTACS) and chemical biology.

Text books:

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

References:

1. Lehninger, Nelson and Cox, *Principles of Biochemistry*, CBS Publishers, 1993.
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.

CH 632 Solid State and Interfacial Chemistry 3 0 0 6

Structure of solids, surfaces and interface, electronic band structures of solids. Electric and magnetic properties of solids: insulators, semiconductors, conductors and superconductor; dielectrics and ferroelectrics; diamagnetism and paramagnetism; ferromagnetism, ferrimagnetism and antiferromagnetism. Diffraction techniques and the structure of solids; Crystal defects, Structure of solid electrolytes, zeolites and conducting polymers and surfaces. Adsorption isotherms; Adsorption on porous solids, chemisorption of gases on metals and semiconductors, kinetics of adsorption processes; surface catalysis: Langmuir-Hinshelwood mechanism. Physical chemistry of colloids,

micelles and macromolecules. Self-assembly. Characterization of solid surface structure and composition using electron microscopy, XPS, Auger, Mossbauer and EELS.

Text books:
1. C. Kittel, *Introduction to Solid State Physics*, 6th Ed., Wiley, 1991.
2. A. R. West, *Solid State Chemistry and Its Applications*, Wiley, 1989.

References:
1. D. K. Chakrabarty, *Adsorption and catalysis by solids*, Wiley Eastern, 1990.
2. F. P. Kane and G. B. Larrabee (Eds.), *Characterisation of solid surfaces*, Plenum, 1978.
3. P. A. Cox, *Electronic Structure and Chemistry of Solids*, Oxford University Press, 1991.
4. G. H. Stout and L. H. Jensen, *X-ray Structure Determination: A Practical Guide*, 2nd Ed., John Wiley, 1989.

Common Elective Courses

CH 603: Concepts for Molecular Machine 3-0-0-6

[Note: This is a new course]

Prerequisite: Fundamentals aspects of spectroscopy

Miniaturization of machines, Terminologies in molecular machine, Energetic and states of molecular machines. Operational aspects and design; Tweezers, Molecular rotors, brake, bevel gear, gyroscopes, Nano-car, Molecules walking, Thermodynamics of interlocked systems, Motions in rotaxanes and catenanes, Switching in rotaxanes, Knots, Molecular elevator, Photochemical switching, photosensitiser, Photochemically driven molecular shuttle, Light driven conformation adjustments, Light-powered molecular pedal, photosensitive liquid crystalline materials, Electrochemically driven machines, Rotations by redox couple; Bio-inspired concepts in molecular machines - Protein synthesis, ATP synthesis; Biological molecular machines for transport - Movement of Kinesins and Dyneins. DNA based tweezers, walker, molecular gear, DNA nano-machine, molecular assembler.

Text books:
1. Credi A, Silvi S, Venturi M, (eds) Molecular Machines and Motors: Recent Advances and Perspectives (2014) *Topics in Current Chem.* Volume 354, Springer, Heidelberg.
2. Baruah JB (2018) Concepts for Molecular machines, World Scientific, Singapore.

Reference:
1. Erbas-Cakmak S, Leigh DA, McTernan CT, Nussbaumer AL (2015) Artificial molecular machines. *Chem. Rev.* **115**: 10081-10206.

CH 614: Supramolecules: Concepts and Applications 3 0 0 6

[Note: The course structure remains as before. Only course number is changed. Old course number was CH 603]

Pre-requisites: Nil

Host design, preorganised hosts, complementarity, Cation, anion and neutral molecule binding hosts. Ionophores, receptors, recognitions, nano-dimensional hosts, supramolecular isomerism. Non-

covalent synthesis, multicomponent cocrystals, synthons, halogen-bonds, pi-interactions, interplay of weak interactions. Clathrates, inorganic solid state clathrates, layered solids, channel structures. Intracavity complexes of neutral molecules, crystal engineering, graph set analysis, conformational polymorphs, co-ordination polymers, liquid crystals. Porous materials, surfactants. Supramolecular approach for chemistry-biology interface, neurotransmitters, optical sensing, switches, enzyme substrate binding, supramolecular catalysis, biominerlisation, hydrophobic confinement in bio-mimicking molecules, MOFs as metalloenzymes.

Texts:

1. J. W. Steedand 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.

Reference:

1. J. L. Atwood, J. E. D. Davies, D. D. McNicol and F. Vogtle (Exe. Ed), Comprehensive Supramolecular Chemistry, Pergamon, New York.

CH 615: Applied Crystallography 3 0 0 6

[Note: The course structure remains as before. Only course number is changed. Old course number was CH 605]

Pre-requisites: Nil

Symmetry and Symmetry operations: 1D, 2D and 3D symmetry, Symmetry in Molecule, Symmetry in Crystal; Crystal: Crystal lattice, Unit cell, Crystal systems, Bravais lattice, Planes in Lattices and Miller Indices, Reciprocal lattice, Postulates of Crystallography (law of constancy of angles, law of rational indices); Crystallographic point groups and Space groups; Crystal growth, Crystal defects and Twining; X-rays: Origin, Production, Absorption, Filtering, Detectors, Selection of radiation, Fundamentals of Diffraction Theory: Diffraction by a 3D-lattice, Bragg's law; Structure determination by X-ray crystallographic method: Choosing a crystal, Shaping a crystal, Crystal mounting, Optical alignment, Data collection, Data reduction, Phase problem, Direct method, Heavy atom method, Absorption correction, Refinement of crystal structures, Completing the structure. Disorders in crystal structures and their applications.

Text Books:

1. G. H. Stout and L. H. Jensen, *X-ray Structure Determination: A Practical Guide*, The Macmillan Company, New York.
2. *Crystal Design: Structure and function*, Ed. G. R. Desiraju, Wiley 2003.
3. Lesley Smart and Elaine Moore, *Solid State Chemistry: An Introduction*, Chapman & Hall 1985.

References:

1. W. Massa, *Crystal Structure Determination*, Springer Verlag, Berlin, 2000.
2. W. Clegg, *Crystal Structure Analysis: Principles and Practice*, Oxford University Press, 2001.
3. *Organic solid-state Chemistry*, Ed. G. R. Desiraju, Elsevier, 1987.
4. J. J. Rousseau, *Basic Crystallography*, John Wiley & Sons, New York, 1998.
5. Jenny P. Glusker, Mitchell Lewis and Miriam Rossi, *Crystal Structure Analysis for Chemists and Biologists*, VCH, New York, 1994.
6. B. D. Cullity and S. R. Stock, *Elements of X - ray diffraction*, Prentice Hall, New Jersey, 2001.

CH 625: Advances in Biological Macromolecules 3-0-0-6

[Note: This is a new course.]

Pre-requisites: Nil

Advances in proteins, solid phase peptide synthesis, synthesis of peptide antibiotics, post-translational 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 lapidated 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.

Text Books:

1. A. Miller and J. Tanner, *Essentials of Chemical Biology*, Willey & 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, J. 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*, Willey & 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. Fruton, *Proteins, Enzymes, Genes: the Interplay of Chemistry and Biology,* (xii 1 783 pages).Yale University Press, 1999.

INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI

MINUTES OF THE 96th MEETING OF THE INSTITUTE POSTGRADUATE PROGRAMME COMMITTEE (IPPC) held on 11 APRIL 2019

CH 631: Advanced Quantum Chemistry 3 0 0 6

[Note: The course structure remains as before. Only course number is changed. Old course number was CH 637]

Pre-requisites: Prior knowledge of Quantum Chemistry

Introduction: Vector interpretation of wavefunction, Hermitian operator, approximate solutions to the Schroedinger 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 self-consistent 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.

Text Books:

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. Szaboa 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.

CH 639: Principles and Applications of Molecular Fluorescence 3 0 0 6

[Note: The course structure remains same as before in all respect.]

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.

Text Books:
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.

DEPARTMENT OF CHEMISTRY
INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI

Departmental Elective Courses for M. Sc./PhD/Common In Chemistry

M. Sc. Elective Courses
(Syllabus as part of newly revised M. Sc. Course structure)

CH 611 Advanced Organometallic Chemistry 3 0 0 6
CH 612 Inorganic Clusters 3 0 0 6
CH 613 Applied Inorganic Chemistry 3 0 0 6
CH 621 Modern Reagents in Organic Synthesis 3 0 0 6
CH 622 Methods in Organic Synthesis 3 0 0 6
CH 623 Supramolecular Chemistry 3 0 0 6
CH 624 Fundamentals of Chemical Biology 3 0 0 6
CH 632 Solid State and Interfacial Chemistry 3 0 0 6
[All the syllabi are placed under the newly revised M.Sc. curriculum with a Note at the bottom. A summary sheet also is provided]

Common Elective Courses

CH 603 Concepts for Molecular Machine 3 0 0 6
CH 614: Supramolecules: Concepts and Applications 3 0 0 6
CH 615: Applied Crystallography 3 0 0 6
CH 625 Advances in Biological Macromolecules 3-0-0-6
CH 631: Advanced Quantum Chemistry 3 0 0 6
CH 639 Principles and Applications of Molecular Fluorescence 3 0 0 6

[All the syllabi are placed under the newly revised M.Sc. curriculum with a Note at the bottom. A summary sheet also is provided]

INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI

MINUTES OF THE 96th MEETING OF THE INSTITUTE POSTGRADUATE PROGRAMME COMMITTEE (IPPC) held on 11 APRIL 2019

Ph. D. Elective Courses

CH 601 Physical Methods in Chemistry 3 – 0 – 0 6
CH 602 Optical and Electronic Materials: A molecular Approach 3 – 0 – 0 6
CH 617 Organometallics 3 – 0 – 0 6
CH 618 Bioinorganic Chemistry 3 – 0 – 0 6
CH 633 Chemical Applications of Group Theory 3 – 0 – 0 6
CH 634 Time Dependent Quantum Mechanics 3 – 0 – 0 6
CH 635 Basic Statistical Mechanics 3 – 0 – 0 6
CH 636 A Fundamental Approach to Physical Chemistry 3 – 0 – 0 6
CH 637 Computational Methods in Chemistry 2-0-2 6
CH 626 Art in Organic Synthesis 3 – 0 – 0 6
CH 627 New Reagents for Organic Synthesis 3 – 0 – 0 6
CH 628 Chemistry of Biological Macromolecules 3 – 0 – 0 6
CH 629 Advances in Bioorganic Chemistry 3 – 0 – 0 6

[All the syllabi are placed below which are total Ph.D. electives with a Note at the bottom. A summary sheet also is provided]

CH 601 Physical Methods in Chemistry 3 – 0 – 0 6

[Note: The course structure/course no. remains the same as before.]

Prerequisite: Nil

Nuclear magnetic resonance spectroscopy: General principles, sensitivity of the method, CW and FT-NMR, 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, 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 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: Theoritical plate concept, van Deemter equation. Gas Chromatography: types of GC, basic components of GC, optimization of the method, GC-MS, Applications. High performance Liquid Chromatography: Different types of HPLC, basic components of HPLC, optimization of methods, 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. Morril, *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.

CH 602 Optical and Electronic Materials: A molecular Approach 3 – 0 – 0 6

[Note: The course structure/course no. remains the same as before.]

Prerequisite: Nil

Overview of electronic devices, band theory, zone theory, conjugated systems, electronic excitation, chromophores, phosphorescence and fluorescence. Theories and application of one dimensional substances: Electron-phonon coupling, Peirerls transition, solitons and polarons, superconductivity, conducting polymers, solution switching, molecular cellular automata, biocomputing, switching molecules, Langmuir Blodgett layers, holographic storage, light emitting diodes; semiconductor devices, defect structures, p, n-type semiconductor, structure property relations in high Tc superconductors. Chemical vapour deposition: Epitaxial growth, crystalline and amorphous films, metal organic vapour deposition, micro and nano crystalline materials, ceramic materials. Electrochemistry of corrosion: thermodynamics of corrosion, electrode kinetics, corrosion mechanism of electronic material systems, corrosion and protection. Fuel cells: operational characteristic, power generation. Lithography: Principle, optical Lithography, deep-UV resists, multi layer systems, top surface imaging systems, plasma etching, dielectric and optical interconnects; biological application of photochemical switches, biosensors, immunoassay, neurotransmitters, fluorescence labels, supramolecular devices, supramolecular electrochemistry, supramolecular ionics, molecular magnets, ion response monolayers, molecular channels, photohysteresis, dual mode photoswitching, self assembly of supramolecular liquid crystalline polymers, supramolecular material and composites.

Texts books:
1. H. B. Pogge and Mercel Dekker (Ed), *Electronic Material Chemistry*, New York, 1996.
2. S. Roth, *One – dimensional metals: Physics and material science,* VCH, New York, 1995.
3.H. Morrission (Ed), *Biological application of photochemical Switches*, John Wiley, New York, 1993.

Reference:
1. J. M. Lehn, *Supramolecular Chemistry: Concept & perspective*, VCH, New York, 1995.
2. C. N. R. Rao and J. Gopalakrishnan, *New Direction in solid state Chemistry*, Cambridge University Press, 1997.
3. R. Arshahy (Ed.), *Desk reference of functional polymers: synthesis and application*; American Chemical Society, Washington, DC, 1996.
4. G. Burns, *High temperature superconductivity an introduction*, Academic press, New York, 1992.

CH 617 Organometallics 3 – 0 – 0 6

[Note: Only course number is changed. Old course number was CH 610]

Prerequisite: Nil

Definition, classifications and bonding in organometallics, isolobal analogies, structural aspects of organometallics, preparative methods. Spectroscopic techniques in organometallics chemistry. Electronic and magnetic properties of organometallic compounds. Stoichiometric and catalytic reactions: Fundamental process 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.

Text books:

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.

CH 618 Bioinorganic Chemistry 3 – 0 – 0 6

[Note: Only course number is changed. Old course number was CH 611]

Prerequisite: Nil

Role of metal ions in Biology: Physiological effects of 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, pKa values of coordinated ligand, redox potential, Nernst equation, some 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 (specially d-d transitions), EPR (emphasis on first row transtion metal ions and their spectra), brief description of CD/MCD and multinuclear NMR. Brief descrieption and capability of newer methods like EXAFS, XANES, ENDOR. Classifications of metalloproteins and enzymes based on function with example: Metalloproteins; Dioxygen transport (Hemoglobin, Hemocyanin), electron transfer (blue cuprotiens, cytochromes, iron-sulphur protein), structural roles (zinc finger), uptake and storage proteins (ferritines). 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 approach employed in solving the problems in bioinorganic chemistry: Use of coordination complexes as 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 role of nitric oxide and other topics will be discussed and student will participate 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.)

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CH 633 Chemical Applications of Group Theory 3 – 0 – 0 6

[Note: Only course number is changed. Old course number was CH 632]

Prerequisite: Nil

Definitions and Theorems of Group Theory: Properties of Group and examples, subgroups, slasses. 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, 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 π bonding, naphthalene. Electronic excitations of naphthalene: Selection rules and configuration interaction, three center bonding. Symmetry based selection rules for cyclization reactions. Molecular Orbital Theory for inorganic and organometallic compounds: Transformation properties of atomic arbitals. Molecular orbitals for σ bonding in AB_n molecules: The Tetrahedral AB_4 cases. Molecular orbitals for π 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.

CH 634 Time Dependent Quantum Mechanics 3 – 0 – 0 6

[Note: Only course number is changed. Old course number was CH 638]

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.

CH 635 Basic Statistical Mechanics 3 – 0 – 0 6

[Note: Only course number is changed. Old course number was CH 643]

Pre-requisites: Nil

Introduction of Statistical Mechanics: Macroscopic states, microscopic states, maximum-entropy principle, determination of the number of microstates, and statistical origin of thermodynamics, Entropy of mixing and the Gibbs correction, Ensemble Theory: Phase space, Liouville's theorem, theory of microcanonical ensemble, Canonical Ensemble Theory: Theory of distribution function for canonical ensemble, statistical quantities in canonical ensemble, ideal gases in canonical ensemble theory, energy fluctuation, equipartition theorem, molecular partition function, translational, rotational, vibrational, electronic and nuclear partition function, concepts of negative temperature, Grand Canonical Ensemble: Distribution function of grand canonical ensemble, statistical quantities in the theory of grand canonical ensemble, Quantum ideal gases: Fermi-Dirac and Bose-Einstein statistics.

Texts:

1. D. A. McQuarrie, Statistical Mechanics, University Science Books, 2000.
2. R. K. Pathria and Paul D. Beale, Statistical Mechanics, Elsevier, 2011.

References:

1. K. Huang, Statistical Mechanics, Wiley, 2008.
2. Y. V. C. Rao, Postulational and Statistical Thermodynamics, Allied Publishers Pvt. Ltd., 1994.

CH 636 A Fundamental Approach to Physical Chemistry 3 – 0 – 0 6

[Note: Only course number is changed. Old course number was CH 630]

Pre-requisites: Nil

Quantum Chemistry: The concept, foundation, postulates and general principles. The Schrödinger wave equation. Application – particle in a box, the harmonic oscillator and the rigid rotor, the hydrogen atom, approximate methods, multielectron atoms, the chemical bond (diatomic to polyatomic). **Spectroscopy:** Basic principles of electronic, vibrational and rotational spectroscopies. Fundamentals of nuclear magnetic resonance (n.m.r.) and electron spin resonance (e.s.r.) spectroscopies. Mossbauer Spectroscopy, Solid state and surface spectroscopies. **Photochemistry:** Fundamentals of Photophysical and photochemical processes. Lasers in photochemistry. **Statistical Thermodynamics:** The Boltzmann Factor and partition functions. Thermodynamic quantities e.g., entropy, Helmholtz and Gibbs Free Energies. **Reaction Dynamics:** Molecular collisions, Scattering, Molecular Energy Transfer and Chemical Reactivity. **Solids and Surface Chemistry:** The unit cell, Symmetry, X-Ray Diffraction in solids. The nature of surfaces compared to the bulk, Physisorption and Chemisorption on surfaces. Reactions on surfaces.

Text Books:

1. Physical Chemistry: A Molecular Approach by Donald A McQuarrie and John D. Simon; Viva Books Private Limited, New Delhi, First South Asian Edition, 1998.

References:

1. Quantum Chemistry; Ira N. Levine, Fourth Edition; Prentice / Hall of India Pvt. Ltd., New Delhi – 1994 (or later).
2. Molecular Reaction Dynamics and Chemical Reactivity by Raphel D. Levine and Richard Bernstein; Oxford University Press; 1987 or later.

3. Dynamics of Molecules and Chemical Reactions by Robert E. Wyatt and John Z. H. Zhang, Marcel Dekker, Inc. New York 1996.
4. Fundamentals of Statistical and Thermal Physics by F. Reif, Mc. Graw Hill, 1985.
5. Molecular Vibrations by E. Bright Wilson, jr., J. C. Decius and Paul C. Cross Dover Publications, Inc., New York 1980.
6. Molecular Rotation Spectra by H. W. Kroto, Dover Publications Inc., New York, 1992.
7. Symmetry and Spectroscopy: An introduction to Vibrational and Electronic Spectroscopy, Daniel C. Harris and Michael D. Bertolucci, Dover Publications Inc., New York, 1978.
8. Fourier Transform N. M. R. spectroscopy by Derek Shaw; Studies in Physical and Theoretical Chemistry Vol. 30, Elsevier 1987.

CH 637 Computational Methods in Chemistry 2-0-2 6

[Note: Only course number is changed. Old course number was CH 634]

Prerequisites : Nil

Introduction to 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.

Text Books :

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, 4th edition, Tata McGraw -Hill, 2002.
5. F. Jensen, Introduction to Computational Chemistry, 3rd edition, Wiley, 2017.

References :

1. V. Rajaraman, Computer Programming in 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.

CH 626: Art in Organic Synthesis 3 – 0 – 0 6

[Note: Old Course is modified and course number is changed. Old course number was CH 620/625]

Pre-requisites: Nil

Retrosynthetic Analysis: Basic for retrosynthetic analysis, Transforms and retrons, Types of Transforms, Biomimitic 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 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 Groupkeyed 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.

CH 627: New Reagents For Organic Synthesis 3 – 0 – 0 6

[Note: Old Course is modified and course number is changed. Old course number was CH 621/627]

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 reagent such as Pyridinium Chloro Chromate, Pyridinium Fluoro Chromate, Swern oxidation, DCC oxidation, Tetrapropyl ammonium peruthenate, other oxidizing agent. Reducing agents: Reductions involving (NaBH) 4, (LiAlH)4, (NaBH)3CN, DIBAL, Red –Al.

Texts:

1. R. O. C Norman and J. H. Coxon, *Principle of Organic Synthesis*, 1st Ed, ELBS, 1993.
2. T. Imamoto, *Lanthenides in Organic synthesis*, Academic Press, 1994.
3. W. Carrutuer, *Some Modern methods of Organic Synthesis*, Cambridge, 1990.
4. L. W. Paqueette (Ed), *Reagents for Organic synthesis*, John Wiley, 1995.

CH 628: Chemistry of Biological Macromolecules 3 – 0 – 0 6

[Note: Old Course is modified and course number is changed. Old course number was CH 623]

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 lapidated 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.

Text Books:

1. C.M. Dobson, J.A. 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, 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*, Willey & Sons Ltd., 2008.

CH 629 Advances in Bio-Organic Chemistry 3-0-0-6

[Note: Old Course is modified and course number is changed. Old course number was CH 641]

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, inhibiton and drug design, enzyme catalysed 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; personalised medicine.

Text Books:

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: http://www.nptel.iitm.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 1 783 pages).

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[SUMMARY SHEET]

Departmental Elective Courses for M. Sc./PhD/Common In Chemistry

M. Sc. Elective Courses
(Syllabus as part of newly revised M. Sc. Course structure)

CH 611 Advanced Organometallic Chemistry 3 0 0 6
CH 612 Inorganic Clusters 3 0 0 6
CH 613 Applied Inorganic Chemistry 3 0 0 6
CH 621 Modern Reagents in Organic Synthesis 3 0 0 6
CH 622 Methods in Organic Synthesis 3 0 0 6
CH 623 Supramolecular Chemistry 3 0 0 6
CH 624 Fundamentals of Chemical Biology 3 0 0 6
CH 632 Solid State and Interfacial Chemistry 3 0 0 6

Common Elective Courses

CH 603 Concepts for Molecular Machine 3 0 0 6
[Note: This is a new course → Syllabus is given].

CH 614: Supramolecules: Concepts and Applications 3 0 0 6
[Note: Only course number is changed. Old course number was CH 603 → Syllabus is given]

CH 615: Applied Crystallography 3 0 0 6
[Note: Only course number is changed. Old course number was CH 605 → Syllabus is given]

CH 625 Advances in Biological Macromolecules 3-0-0-6
[Note: This is a new course → Syllabus is given]

CH 631: Advanced Quantum Chemistry 3 0 0 6
[Note: Only course number is changed. Old course number was CH 637 → Syllabus is given]

CH 639 Principles and Applications of Molecular Fluorescence 3 0 0 6
[Note: The course structure/course no. remains the same as before → Syllabus is given]

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Ph. D. Elective Courses

CH 601 Physical Methods in Chemistry 3 – 0 – 0 6
[Note: The course structure/course no. remains the same as before. → Syllabus is given]

CH 602 Optical and Electronic Materials: A molecular Approach 3 – 0 – 0 6
[Note: The course structure/course no. remains the same as before. → Syllabus is given]

CH 617 Organometallics 3 – 0 – 0 6
[Note: Only course number is changed. Old course number was CH 610→ Syllabus is given]

CH 618 Bioinorganic Chemistry 3 – 0 – 0 6
[Note: Only course number is changed. Old course number was CH 611→ Syllabus is given]

CH 633 Chemical Applications of Group Theory 3 – 0 – 0 6
[Note: Only course number is changed. Old course number was CH 632→ Syllabus is given]

CH 634 Time Dependent Quantum Mechanics 3 – 0 – 0 6
[Note: Only course number is changed. Old course number was CH 638→ Syllabus is given]

CH 635 Basic Statistical Mechanics 3 – 0 – 0 6
[Note: Only course number is changed. Old course number was CH 643→ Syllabus is given]

CH 636 A Fundamental Approach to Physical Chemistry 3 – 0 – 0 6
[Note: Only course number is changed. Old course number was CH 630→ Syllabus is given]

CH 637 Computational Methods in Chemistry 2-0-2 6
[Note: Only course number is changed. Old course number was CH 634→ Syllabus is given]

CH 626 Art in Organic Synthesis 3 – 0 – 0 6
[Note: Old Course is modified and course number is changed. Old course number was CH 620/625→ Syllabus is given]

CH 627 New Reagents for Organic Synthesis 3 – 0 – 0 6
[Note: Old Course is modified and course number is changed. Old course number was CH 621/627→ Syllabus is given]

CH 628 Chemistry of Biological Macromolecules 3 – 0 – 0 6
[Note: Old Course is modified and course number is changed. Old course number was CH 623→ Syllabus is given]

CH 629 Advances in Bioorganic Chemistry 3 – 0 – 0 6
[Note: Old Course is modified and course number is changed. Old course number was CH 641→ Syllabus is given]

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