UNIVERSITY OF KERALA

DEPARTMENT OF CHEMISTRY

M.Sc. PROGRAMME IN CHEMISTRY

(Under Credit and Semester System w.e.f. 2013 Admission)

The programme shall extend over a period of two academic years comprising of four semesters each of 5 months duration.

CURRICULUM STRUCTURE

Course No.	Course Title	Contact hours per week			No. of Credits
		Lec	*Tut*	*Lab*	
	SEMESTER I				
Core courses					
CHE 511	Periodic Table – Elements and Properties	3	1	0	3
CHE 512	Reaction Mechanisms and Stereochemistry	3	1	0	3
CHE 513	Theoretical Chemistry	3	1	0	3
CHE 514	Inorganic Chemistry Lab-I	0	0	6	2
CHE 515	Organic Chemistry Lab-I	0	0	6	2
CHE 516	Physical Chemistry Lab-I	0	0	6	2
Elective courses					
	Extra departmental courses	3	0	0	3
	Total	**12**	**3**	**18**	**18**
	SEMESTER II				
Core courses:					
CHE 521	Coordination Chemistry	3	1	0	3
CHE 522	Symmetry and Organic Spectroscopy	3	1	0	3
CHE 523	Kinetics and Spectroscopy	3	1	0	3
CHE 524	Inorganic Chemistry Lab-II	0	0	6	2
CHE 525	Organic Chemistry Lab-II	0	0	6	2
CHE 526	Physical Chemistry Lab-II	0	0	6	2
Elective courses					
	Extra departmental courses	3	0	0	3
	Total	**12**	**3**	**18**	**18**

SEMESTER III

Core courses:					
CHE 531	Solid State and Organometallic Chemistry	3	1	0	3
CHE 532	Organic Synthesis and Bioorganic Chemistry	3	1	0	3
CHE 533	Surface Chemistry, Electrochemistry and Thermo dynamics	3	1	0	3
CHE 534	Inorganic Chemistry Lab-III	0	0	6	2
CHE 535	Organic Chemistry Lab-III	0	0	6	2
CHE 536	Physical Chemistry Lab-III	0	0	6	2
Elective courses:					
CHE 501	Advanced Inorganic Chemistry	3	0	0	3
CHE 502	Advanced Organic Chemistry	3	0	0	3
CHE 503	Advanced Physical Chemistry	3	0	0	3
	Total	**12**	**3**	**18**	**18**

** Each student must select one elective among the three electives CHE 501-3 given above .*

SEMESTER IV

Core courses:					
CHE 541	Analytical Principles and Environment	4	1	0	4
CHE 542	Instrumental Methods	4	1	0	4
CHE 543	Dissertation	0	0	18	6
Elective courses:					
CHE 504	Applied Chemistry	3	1	0	4
CHE 505	Applied Electrochemistry	3	1	0	4
CHE 506	Chemistry of Nanomaterials	3	1	0	4
CHE 507	Electronic Structure Theory and Applications	3	1	0	4
CHE 508	Photophysical Processes and Applications	3	1	0	4
CHE 509	Organic Synthesis	3	1	0	4
	Total	**11**	**3**	**18**	**18**

**Each student must select one elective among the six electives CHE 504-9 given above*

Grand Total	**47**	**12**	**72**	**72**

Total credits for cores: 35 (theory) + 18 (labs) + 6 (dissertation); electives: 13

TOTAL CREDITS= 72

UNIVERSITY OF KERALA
DEPARTMENT OF CHEMISTRY
SYLLABUS FOR M.Sc. PROGRAMME IN CHEMISTRY
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SEMESTER I

Core courses

CHE 511 PERIODIC TABLE – ELEMENTS AND PROPERTIES 3 Credits

Unit I Main Group Elements

Chemistry of the noble gases: Xenon fluorides and oxofluorides. Xenon compounds with bonds to other elements. Chemistry of Krypton and Radon. Chemistry of halogens: Halogens in positive oxidation states. Interhalogen compounds, pseudohalogens and polyhalide ions. Astatine.

Unit II Transition Metals

Survey of the transition elements. General characteristics of transition elements. Oxidation states. Study of the following groups of elements and their compounds with peculiar structures and their chemistry:

Ti	V	Cr	Mn
Zr	Nb	Mo	Tc
Hf	Ta	W	Re

Polyacids: Isopoly and heteropoly acids of Mo and W. Structure and properties of refractory and ionic borides, carbides, nitrides and silicides. Silicates: Classification and structure. Silicones.

Unit III- Lanthanides and Actinides

Lanthanides: Characteristic properties. Electronic configuration, Occurrence and extraction. Separation techniques. Oxidation states. Spectral and magnetic properties. Actinides: Occurrence and general properties. Electronic configuration, Oxidation states. Spectral and magnetic properties. Comparative properties of lanthanides and actinides. Trans-uranium elements and their stabilities. Applications of lanthanides, actinides and their compounds.

Unit IV Rings, Cages and Clusters

Boron hydrides: Reactions of diborane, structure and bonding. Polyhedral boranes: Preparation, properties, structure and bonding. The topological approach to boron hydride structure. Styx numbers. Wade's rules. Carboranes: Closo, nido and arachno carboranes. Metallaboranes and metallacarboranes. Organoboron compounds and hydroboration. Boron-nitrogen compounds: Borazine, substituted borazines and boron nitride, S, N and P compounds, Sulphur-Nitrogen compounds: Tetrasulphur tetranitride, disulphur dinitride and polythiazyl. S_xN_y compounds. S-N cations and anions. Other S-N compounds. Sulphur-phosphorus compounds: Molecular sulphides such as P_4S_3, P_4S_7, P_4S_9 and $P_4S_{10.}$ Phosphorus-nitrogen compounds: Phosphazines. Cyclo and linear phosphazines. Other P-N compounds.

References

1. F.A. Cotton and G. Wilkinson, "Advanced Inorganic Chemistry", 6th Edn, Wiley Interscience, New York, 1999.
2. James E.Huheey, Ellen A. Keiter and Richard L.Keiter, "Inorganic Chemistry - Principles of Structure and Reactivity", 4th Edn, HarperCollins, New York., 1993.

3. B.E.Douglas, D.H.McDanial and J.J.Alexander, “Concepts and Models of Inorganic Chemistry”, 3rd Edn, John Wiley, 2001.
4. H. J. Emeleus and A. G. Sharpe, “Modern Aspects of Inorganic Chemistry”, Universal Book.
5. S. S. A. Cotton, "Lanthanides and Actinides", Macmillan. London, 1991.
6. K. F. Purcell and J. C. Kotz, “Inorganic Chemistry”, Saunders.

Further Reading

1. P. W. Atkins and D. F. Shriver, “Inorganic Chemistry”, 5th Edn, OUP.
2. A. F. Holleman and E. Wiberg, “Inorganic Chemistry”, Academic.

CHE 512 REACTION MECHANISMS AND STEREOCHEMISTRY 3 Credits

Unit I Structure and Stereochemistry

Correlation of structure and reactivity, Effects of structure on acidity, basicity and reactivity, Kinetic and thermodynamic control of reactions. Hammond’s postulate. Hammett and Taft equations, Concept of aromaticity. Aromaticity of annulenes, mesoionic compounds, metallocenes, cyclic carbocations and carbanions. Non-benzenoid aromatics, Fullerenes. Molecular chirality, stereochemical nomenclature of compounds with chiral centres, axis and planes, prostereoisomerism, stereotopicity and stereoprojections. Non-carbon chiral centres. Atropisomerism and its designation. Stereoselective and stereospecific reactions, regioselective and regiospecific reactions, enantiomeric excess and chiral separation methods. Conformational analysis of alkanes, cycloalkanes and biased systems. Effect of conformation on reactivity of cyclohexane and decalin derivatives.

Unit II Reactions of sp^3 Carbon Systems

Stereochemical and mechanistic aspects of S_N reactions. Effect of solvent, leaving group and substrate structure. Neighbouring group participation. Nonclassical carbocations and ion pairs in S_N reactions. Ambident nucleophiles and substrates. S_N' and S_Ni reactions. Isotopic and salt effects, Elimination reactions leading to C=C bond formation. E1, E2 and E1cB mechanisms. Hoffman and Saytzeff modes of elimination. Effect of leaving group and substrate structure. Cis eliminations.

Unit III Reactions of sp^2 Carbon and Aromatic Systems

Electrophilic addition to C=C: Reactions and their mechanistic and stereochemical aspects. C=O based and C=O activated reactions. Named reactions based on C=O group. Stereochemistry of addition to C=O systems. Cram's rule. Felkin-Anh Model. Mechanism of esterification and ester hydrolysis. Aromatic electrophilic and nucleophilic substitutions. Electronic and steric effects of substituents. S_N1, S_NAr, Benzyne and $S_{RN}1$mechanism and their evidences. Radical additions, substitutions and chain reactions.

Unit IV Reactive Intermediates and Rearrangement Reactions

Intermediates in organic synthesis. Structure, stability, formation and reactions of carbenes, nitrenes, benzynes, carbon radicals, carbocations, carbanions, radical-ions and ylides, Named reactions and mechanisms involving all these species. Types of organic rearrangements. Anionotropic, cationotropic, prototropic, radical, carbene, nitrene and long-range rearrangements. Migratory aptitude in rearrangements. Rearrangements involving C → C, C → N, C → O, hetero atom → C migrations of H, alkyl, aryl, hetero atom and other groups.

References

1. Francis A.Carey and Richard J. Sundberg, “Advanced Organic Chemistry - Part A: Structure and Mechanisms”, 5th Edn, Springer, 2007.
2. P. Y. Bruice, "Organic Chemistry", 6th Edn, Prentice Hall
3. M. B. Smith and J. March, "March’s Advanced Organic Chemistry", 6th Edn, Wiley. 2007.

4. D. Nasipuri, "Stereochemistry of Organic Compounds", 2nd Edn, Wiley Eastern, 1994.
5. T. H. Lowry and K. S. Richardson, “Mechanism and Theory in Organic Chemistry” 3rd Edn, Harper Row, 1987.

Further Reading

1. P. Sykes, "A Guidebook to Mechanisms in Organic Chemistry", 6th Edn, Longman, 1986.
2. P. S. Kalsi, "Stereochemistry and Reaction Mechanisms", 1993, Wiley Eastern.
3. J. Clayden, N. Geeves, S. Warren, “Organic Chemistry”, OUP.
4. C. J. Moody and W.H. Whitham, "Reactive Intermediates", 1992, OUP.
5. S. N. Issacs, "Physical Organic Chemistry", Longman.
6. L. G. Wade, “Organic Chemistry 5 Edn, Prentice Hall
7. F. A. Carey and R.J. Sundberg. "Advanced Organic Chemistry Part A:, 4 Edn. Kluwer
8. F. A. Carroll, “Perspectives on Structure and Mechanism in Organic Chemistry”, Brooks Cole
9. R. Bruckner, “Advanced Organic Chemistry”, Harcourt-Academic.
10. M. A. Fox and J. K. Whitesell, “Organic Chemistry”, 3 Edn, Jones Bartlett

CHE 513 THEORETICAL CHEMISTRY 3 Credits

Unit I Quantum Mechanics-1

Historic evolution of quantum mechanics: The wave nature of sub-atomic particles. The uncertainty principle and its consequences. The postulates of quantum mechanics. Wave functions, well-behavedness, Orthogonality theorem. Orthonormality. Concept of operators: Laplacian, Hamiltonian, linear and Hermitian operators. Angular momentum operators and their properties. Commutators. Eigen function and eigen values. Expectation value. Time dependent and independent Schrodinger equation.
Solutions of Schrodinger wave equations for:

1. A free particle in 1D. Particle in 1D box of infinite and finite potential wells. Tunnelling. Particle in 3D box. Zero point energy and significance
2. 1D- Harmonic oscillator. Hermite equation and Hermite polynomials. Recurrence formula. Introduction to 3D harmonic oscillator. Oscillator model and Molecular vibrations. Selection rule for vibrational transitions

Unit II Quantum Mechanics-II

Schrodinger equation in polar coordinates. Solutions of Schrodinger wave equations for

1. Rigid rotator. Particle on a ring. Separation of variables. Real and Imaginary Wave functions.
2. Non-planar rigid rotator. Legendre and Associated Legende equations and polynomials. Rodrigue’s formula. Spherical Harmonics. Polar Diagrams. Salient features. Space quantization.
3. Hydrogen atom. Laguerre and Associated Laguerre equations and corresponding polynomials. Space quantization. Spin of electron. Orbitals and Spin orbitals. Radial probability distribution function and graphs. Selection rules for spectral transitions.

Unit III Chemical Bonding

Many body problems. Approximations. Independent particle model. Variational method. Theorem and proof. Variational treatment of hydrogen and helium atom. Secular determinant. Perturbation method. Application to particle in 1-D box of increasing potential, Helium atom. self-consistent field method. Hartree equations and Hartree-Fock equations. Pauli’s exclusion principle. Symmetry and antisymmetry wave functions. Slater determinants. Roothaan equations. Hartree Fock Roothan equations. Vector atom model. Spin orbit coupling. Term symbols and spectral lines.
Molecular problems. Born-Oppenheimer approximation. Valence Bond theory (H2). Molecular Orbital Theory. Ab initio methods. MO theory of hydrogen molecule ion. Electron density distribution and stability of H_2^+ ion. MO theory of homonuclear diatomic molecules. Bond order and stability. MO theory of simple heterogeneous diatomic molecules like HF, LiH, CO and NO.

Semi empirical MO treatment of planar conjugated molecules. Huckel MO theory and calculation of energy of ethylene, butadiene and allylic anions and cyclic systems. Directed valences: The hybridization. Expression for hybrid orbitals in terms of wave functions of s and p orbitals and explanation for directed valences of sp, sp^2 and sp^3 hybrid orbitals.

Unit IV Introduction to Group Theory

Symmetry and character tables: Symmetry elements and symmetry operations. Point groups. Multiplication of operations. Conditions for a set of elements to form a group. Group multiplication table. Similarity transformation and classification of symmetry operations. Matrix representation of point group. Reducible and irreducible representations. Character of a matrix. Orthogonality theorem. Rules derived from orthogonality theorem (proof not required). Setting up of the character tables of simple groups such as C_{2V} and C_{3V} on the basis of the rules. The four areas of the character table. Reduction of reducible representations to irreducible representations. Applications of character tables to spectroscopy. Transition moment operators. Application of character table to orbitals. Construction of hybrid orbitals. Symmetry adapted LCAO.

References

1. I. N. Levine, "Quantum Chemistry", 6th Edition, Pearson Education Inc., 2009.
2. D. A. McQuarrie, "Quantum Chemistry", University Science Books, 1983.
3. L. Pauling and E. B. Wilson, “Introduction to Quantum Mechanics”, McGraw Hill., 1935.
4. H. Jaffe and M. Orchin, "Symmetry in Chemistry", Wiley.
5. F. A. Cotton, "Chemical Applications of Group Theory", Wiley.

Further Reading

1. M. W. Hanna, "Quantum Mechanics in Chemistry", 2nd Edition, W. A. Benjamin. Inc. 1969
2. A. K.Chandra, "Introduction to Quantum Mechanics", 4th Edition, Tata McGraw-Hill. 1994.
3. R. K. Prasad, “Quantum Chemistry”, 3rd Edition, New Age International, 2006.
4. V. Ramakrishnan and M.S. Gopinathan, "Group Theory in Chemistry" , Vishal Publications.

CHE 514 INORGANIC CHEMISTRY LAB-I 2 Credits

1. Separation and identification of rare/less familiar metal ions such as Ti, W, Se, Mo, Ce, Th, Zr, V, U and Li in their binary mixtures. A student must analyse at least 6 samples.
2. Volumetric estimations using EDTA, ammonium vanadate, cerium(IV) sulphate, chloramine-T and potassium iodate. A student must do at least 8 estimations.

References

1. A. I. Vogel, "A Text Book of Qualitative Inorganic Analysis", Longman.
2. A. I. Vogel, “A Text Book of Quantitative Inorganic Analysis", Longman.
3. D. A. Skoog and D. M. West, "Analytical Chemistry: An Introduction", Saunders.

CHE 515 ORGANIC CHEMISTRY LAB-I 2 Credits

1. Quantitative wet chemistry separation of a mixture of two components by solvent extraction [Assessment is based on % recovery].
2. Separation of binary mixtures of organic compounds using chromatographic methods: TLC and column chromatography. Identification using R_F values. [Assessment is based on quality of eparation and/or % recovery].

References

1. C. E. Bell, D. F. Taber and A. K. Clark, “Organic Chemistry Laboratory”, Thomson.

2. D. J. Pasto, C.R. Johnson and M. J. Miller, “Experiments and Techniques in Organic Chemistry”, Prentice Hall.
3. V. K. Ahluwalia and R. Aggarwal, “ Comprehensive Practical Organic Chemistry” Vol 1 & 2, Universities Press.

CHE 516 PHYSICAL CHEMISTRY LAB-I 2 Credits

1. Distribution law: Partition of iodine, ammonia and aniline between water and organic solvents. Association of benzoic acid. Equilibrium constants of tri-iodide and copper-ammonium complexes. Enthalpy change for tri-iodide formation.
2. Refractometry: Refractive index and molar refraction of liquids. Atomic refractions. Composition of solid solutes. Molecular and ionic radii from molar refraction. Study of the complex $K_2[HgI_4]$.
3. Chemical kinetics: Acid hydrolysis of esters. Comparison of strengths of acids. Saponification of esters. Persulphate-iodide second order reaction.Aactivation energy. Arrhenius parameters. Primary salt effect.
4. Thermochemistry: Determination of water equivalent. Heat of neutralization and heat of ionization. Integral and differential heats of solution. Thermometric titrations. Determination of concentrations of strong acids.
5. Polarimetry: Inversion of cane sugar. Velocity constants for different acid strengths. Comparison of strengths of two acids.
6. Adsorptoin: Verification of Langmuir and Freundlich isotherms for solute adsorption on solids. Estimation of surface area. First order kinetics. Computation of adsorption thermodynamics. Exothermic and endothermic reactions.

References

1. A. Finlay and J. A. Kitchener, "Practical Physical Chemistry", Longman.
2. F. Daniels and J. H. Mathews, "Experimental Physical Chemistry", Longman.
3. A. M. James, "Practical Physical Chemistry", Churchill.
4. H. H. Willard, L. L. Merritt and J. A. Dean, "Instrumental Methods of Analysis", East-West.
5. D. P. Shoemaker and C. W. Garland, "Experimental Physical Chemistry", McGraw Hill.

SEMESTER II

Core courses:

CHE 521 COORDINATION CHEMISTRY 3 Credits

Unit I Introduction to Coordination Chemistry

Types of ligands and complexes. Coordination number and geometry. Isomerism: Geometrical, optical and structural isomerism. Stability of complex ions in aqueous solution: Formation constants. Stepwise and overall formation constants. Factors affecting stability of complexes. Determination of stability constants. Chelate and macrocyclic effects.

Unit II Theories of Metal Complexes

Valence bond theory and its limitations. Ligand field theory: Splitting of d orbitals in different ligand fields such as octahedral, tetragonal, square planar, tetrahedral, trigonal bipyramidal and square pyramidal fields. Jahn-Teller effect. LFSE and its calculation. Thermodynamic effects of LFSE. Factors affecting the splitting parameter. Spectrochemical series. Molecular orbital theory based on group theoretical approach and bonding in metal complexes. MO diagrams of complexes with and without π bonds. Effect of π bond on the stability of σ bond. Nephelauxetic series.

Unit III Spectral and Magnetic Properties of Metal Complexes

Spectral properties of complexes: Term symbols for d-ions. Characteristics of d-d transitions. Selection rules for d-d transitions. Orgel diagrams. Tanabe-Sugano diagrams. Effects of Jahn-Teller distortion and spin-orbit coupling on spectra. Charge transfer spectra. Magnetic properties of metal complexes: Types of magnetism shown by complexes. Magnetic susceptibility measurements. Gouy method. Spin-only value. Orbital contribution to magnetic moment. Ferromagnetism and antiferromagnetism in complexes. Application of magnetic measurements to structure determination of transition metal complexes.

Unit IV Reactions of Metal Complexes

Kinetics and mechanism of reactions involving complexes in solution. Inert and labile complexes. Ligand displacement (substitution) reactions in octahedral and square planar complexes. The trans effect. Ligand field effects on reaction rate. Influence of acid and base on reaction rate. Racemization and isomerization. Redox reactions in complexes: Electron transfer and electron exchange reactions. Outer sphere and inner sphere mechanisms of redox reactions.

References

1. F. A. Cotton and G. Wilkinson, “Advanced Inorganic Chemistry”, Wiley.
2. J. E. Huheey, “Inorganic Chemistry: Principles of Structure and reactivity”, Harper Collins
3. D. Banergea, “Coordination Chemistry”, Tata McGraw Hill.
4. A. F. Holleman and E. Wiberg, “Inorganic Chemistry”, Academic.
5. S. F. A. Kettle, "Coordination Chemistry", Longman.

Further Reading

1. E. Lewis and R. G. Wilkins (Eds.), "Modern Coordination Chemistry", Interscience.
2. J. C. Bailar, "Chemistry of Coordination Compounds", Reinhold.
3. D. Banergea, “Coordination Chemistry”,Tata McGraw Hill.

CHE 522 SYMMETRY AND ORGANIC SPECTROSCOPY 3 Credits

Unit I Symmetry Controlled Reactions

Symmetry properties of MOs. Principle of conservation of orbital symmetry. Theory, mechanism and stereocourse of electrocyclic, cycloaddition and sigmatropic reactions, 1,3-dipolar cycloadditions, ene reactions, cheletropic reactions, Sommelet, Hauser Cope, Claisen rearrangements, and thermal eliminations. Woodward-Hoffmann selection rules. secondary orbital interactions in [4+2] cycloadditons, rates of cycloaddition reactions, Fluxional molecules.

Unit II Organic Photochemistry

Primary photoprocesses. Photoreactions of C=O systems, enes, eneones, dienes and arenes. Photoisomerisations, Norrish type I and II reactions. Patterno-Buchi and Barton reactions. Di-π-methane and aromatic photo rearrangements. Photochemical remote functionalisation and hydrogen abstraction reactions. Introduction to PET, chemi and bioluminescent reactions. Chemistry of singlet oxygen. Photochemistry in nature. Photosynthesis. Introduction to organic applied photochemistry and femtochemistry.

Unit III NMR Spectroscopy

^{1}H and ^{13}C NMR chemical shifts and coupling constants of organic compounds. Field and anisotropic factors. Coupled spin systems. Structure implications of δ and J values. Spin systems and their analysis. Tree diagram. Chemical exchange, double resonance, NOE and DEPT. Introduction to 2D NMR. Correlation, NOE and quantum correlation spectroscopy techniques.

Unit IV Organic Structure by Spectroscopy

UV-VIS spectra of enes, eneones, arenes and conjugated systems. Woodward-Fieser rules, Solvent effect on absorption spectra. Characteristic IR bands of functional groups. Identification of functional groups and other structural features by IR. MS in organic structure analysis. EI, CI, FAB, ES and MALDI ion production methods. Characteristic EIMS fragmentation modes and MS rearrangements. Spectral interpretation, structure identification and solving of structural problems using numerical and spectral data.

References

1. I. Flemming, "Frontier Orbitals and Organic Chemical Reactions", John Wiley, 1998.
2. H. Arora, "Organic Photochemistry and Pericyclic Reactions", Wiley Eastern
3. J. M. Coxon and B. Holton, "Organic Photochemistry", CUP.
4. D. H. Williams and I. Flemming, "Spectroscopic Methods in Organic Chemistry", 4th Edition, McGraw-Hill.
5. D.L. Pavia, G.M. Lampman and G.S. Kriz "Introduction to Spectroscopy" 3rd Edition, Brooks/Cole, 2001.

Further Reading

1. Mc Murry, "Organic Chemistry", Thomson Brooks/Cole, 1999.
2. M. Page and A. Williams , "Organic and Bio-organic Mechanisms". Longman.
3. J. J. Li, "Name reactions", 2 Edn, Springer
4. Norman and Coxon, "Organic Synthesis", CRC Press, 3rd En, 1993.
5. C. E. Wayne and R. P. Wayne, "Photochemistry", OU Primer 39, OUP.
5. W. Kemp, "Organic Spectroscopy", Longman.
6. R. M. Silverstein et al., "Spectrometric Identification of Organic Compounds" 6 Edn, Wiley.
7. P. S. Kalsi, "Organic Spectroscopy", Wiley Eastern.
8. J. Kagan, "Organic Photochemistry, Principles and Applications", Academic.
9. P. Suppan, "Chemistry and Light", RSC.
10. J. D. Coyle, "Photochemistry in Organic Synthesis", RSC.

CHE 523 KINETICS AND SPECTROSCOPY 3 Credits

Unit I Chemical Kinetics I: Reaction Rate theories and Thermal reactions

Brownian movement. Determination of Avogadro number. Distribution of molecular velocities. Maxwells equation. Average and most probable velocities from Maxwells equation. Influence of temperature. Thermal conductivity and diffusion. Determination of viscosity of gases. Influence of temperature and pressure on transport properties. Mean free path. Collision diameter. Collision Theory. Activated complex theory. Potential energy surface.

Order and molecularity of reactions. Time dependency of order. Complex reactions: Reversible, consecutive, concurrent and branching reactions. Free radical and chain reactions. Steady state treatment. Reactions like H_2-Cl and H_2-Br_2. Decomposition of ethane, acetaldehyde and N_2O_5. Rice-Herzfeld mechanism. Unimolecular reaction. Lindemann treatment. Semenoff-Hinshelword mechanism of chain reactions and explosion. Kinetics of fast reactions: Relaxation method. Relaxation spectrometry. Flow method. Shock method. Fast mixing method. Field-jump method. Pulse method. Flash photolysis. Factors influencing reaction rates in solution. Salt effects. Curtin-Hammett equation.

Unit II Chemical Kinetics II- Catalysis and Photochemical reactions.

Catalysis: Mechanism and theories of homogeneous and heterogeneous catalysis. Acid-base and enzyme catalysis. Unimolecular and Bimolecular surface reactions. Langmuir-Hinshelwood mechanism

Introduction to photochemistry: Laws of photochemistry. Quantum yield. Radiative and non-radiative transitions. Fluorescence and phosphorescence. Intensity and concentration. Fluorescence indicators. Quenching of fluorescence. Chemiluminescence. Explosion reaction. Kinetics of photochemical reaction of H_2 and Cl_2, and H_2 and Br_2. photopolymerization.

Unit III Spectroscopy-1

Basics of molecular spectroscopy, Microwave spectroscopy. Rotation of diatomic molecules. Rotational spectrum. Intensity of spectral lines. Calculation of internuclear distance. Nonrigid rotors and centrifugal distortion. Introduction to instrumentation. Infrared spectroscopy: Rotational spectra of polyatomic molecules. Linear and symmetric top molecules. Vibrational spectra of harmonic and anharmonic diatomic molecules. Fundamental and overtones. Determination of force constants. Interaction of rotation and vibration. Different branches of spectrum. Symmetry of vibrational-rotation spectrum. Vibrational spectra of polyatomic molecules. Normal modes. Classification of vibrations. Overtones, combination and Fermi resonance. Group frequencies. Introduction to instrumentation and FT IR.

Raman spectra: Scattering of light. Raman scattering. Polarizability and classical theory of Raman spectrum. Quantum theory of Raman spectrum. Rotational and vibrational Raman spectrum. Introduction to instrumentation. Laser Raman spectrum. Raman spectra of polyatomic molecules. Complementarity of Raman and IR spectra.

Unit IV Spectroscopy-2

Electronic spectra: Term symbols of molecules. Electronic spectra of diatomic molecules. Vibrational coarse structure and rotational fine structure of electronic spectrum. Franck-Condon principle. Types of electronic transitions. Fortrat diagram. Predissociation. Morse function. Calculation of heat of dissociation. Introduction to instrumentation.

Electronic spectra of polyatomic molecules: Electronic transitions and absorption frequencies. Effect of conjugation. Resonance spectroscopy: Nuclear spin and interaction with an applied magnetic field. Nuclear resonance. Population of energy levels. ^1H NMR spectrum. Chemical shift. Spin-spin coupling. Fine structure. NMR spectra of other nuclei. Introduction to instrumentation.

Electron spin in molecules and its interaction with magnetic field. ESR spectrum. The g factor and its determination. Fine structure and hyperfine structure. Mossbauer spectroscopy: Doppler effect. Chemical shift. Quadrupole effect.

References

1. G. M. Panchenkov and V.P. Labadev, "Chemical Kinetics and Catalysis", MIR Publishing.
2. E. A. Moelwyn-Hughes, "Chemical Kinetics and Kinetics of Solution", Academic.
3. G. M. Barrow, "Molecular Spectroscopy", McGraw Hill.
4. C. N. Banwell, Fundamentals of Molecular Spectroscopy", McGraw-Hill.
5. F. Daniels and R. A. Alberty, "Physical Chemistry", Wiley Eastern.

Further Reading

1. E. A. Moelwyn Hughes, "Physical Chemistry", Pergamon.
2. P. W. Atkins, "Physical Chemistry", OUP.
3. R. S. Drago, "Physical Methods in Inorganic Chemistry", Reinhold.
4. F. Daniels and R. A. Alberty, "Physical Chemistry", Wiley Eastern.
5. E. A. Moelwyn Hughes, "Physical Chemistry", Pergamon.
6. J. Rose, "Dynamic Physical Chemistry", Issac Pitman.

CHE 524 INORGANIC CHEMISTRY LAB -II **2 Credits**

1. Colorimetric determinations of Cr, Fe, Mn, Ni, Ti, W and Cu.
2. Estimation of simple binary mixtures of metal ions in solution (involving quantitative separation) by volumetric and gravimetric methods.
3. Analysis of some typical alloys such as brass, bronze and type metal.

References

1. A. I. Vogel, "A Textbook of Quantitative Inorganic Analysis", Longman.
2. D. A. Skoog and D. M. West, "Analytical Chemistry: An Introduction", Saunders.
3. I. M. Kolthoff, V. J. Elving and Sandell, "Treatise on Analytical Chemistry", Interscience.
4. Furman and Welcher, "Standard Methods of Inorganic Analysis", Van Nostrand.

CHE 525 ORGANIC CHEMISTRY LAB-II **2 Credits**

1. Preparation of organic compounds by multi-step reactions involving nitration, halogenation, acetylation and oxidation. [Assessement is based on yield and purity].
2. Spectral interpretation of organic compounds [simple as well as prepared in lab as above}using UV-VIS and IR. [Assessement is based on identification and interpretaion].

References

1. B. S. Furniss and others, "Vogel's Textbook of Practical Organic Chemistry" ELBS.
2. V. K. Ahluwalia and R. Aggarwal, " Comprehensive Practical Organic Chemistry" Vol 1 & 2, Universities Press.
3. D. J. Pasto, C.R. Johnson and M. J. Miller, "Experiments and Techniques in Organic Chemistry", Prentice Hall.

CHE 526 PHYSICAL CHEMISTRY LAB -II **2 Credits**

1. Viscosity: Viscosities of liquids and mixtures of liquids. Verification of Kendall's equation and Jones-Dole equation. Viscosity of polymer solutions. Variation of viscosity with temperature.
2. Surface tension: Surface tension and parachor of liquids by differential capillary and stalagmometer methods. Variation of surface tension with concentration. Determination of atomic parachor.
3. Cryoscopy: Determination of molar freezing points. Depression constant and molecular mass using solid and liquid solvents. Study of dissociation and association of solutes. Atomicity of substances like sulphur.
4. Phase equilibria: CST of phenol-water system. Determination of unknown concentrations of NaCl, acetic and oxalic acid. Construction of phase diagrams of unknown mixtures. Three component systems with one pair of partially miscible liquids. Construction of phase diagrams and tie lines. Composition of homogeneous mixtures.
5. Transition temperature: Transition temperature of sodium acetate. K_f of sodium acetate. Molecular mass of urea. Transition temperature of sodium thiosulphate.

References

1. A. Finlay and J. A. Kitchener, "Practical Physical Chemistry", Longman.
2. F. Daniels and J. H. Mathews, "Experimental Physical Chemistry", Longman.
3. A. M. James, "Practical Physical Chemistry", J. A. Churchill.
4. D. P. Shoemaker and C. W. Garland, "Experimental Physical Chemistry", McGraw Hill.
5. J. B. Yadav, "Advanced Practical Chemistry", Goel Publishing House.

SEMESTER III

Core courses:

CHE 531 SOLID STATE AND ORGANOMETALLIC CHEMISTRY 3 Credits

Unit I Introduction to Solid State

Crystal systems and lattice types. Bravais lattices. Crystal symmetry. Point groups and space groups. Miller indices. Reciprocal lattice concept. Close packed structures: BCC, FCC and HCP. Voids. Coordination number. X-Ray diffraction by crystals: Functions of crystals. Transmission grating and reflection grating. Braggs equation. Diffraction methods. Powder, rotating crystal, oscillation and Weisenberg methods. Indexing and determination of lattice type and unit cell dimensions of cubic crystals. Structure factor. Fourier synthesis:

Unit II Solid State – Theories and Properties

Binding forces in solids: Ionic bonding and potential energy field. Lattice energy. Born theory and Born-Haber cycle. Molecular, ionic, covalent, metallic and hydrogen bonded crystals. Free electron theory and band theory of solids. Conductors, insulators and semiconductors. Mobility of charge carriers. Hall effect. Crystal defects: Point, line and plane defects. Electrons and holes. Imperfections and nonstoichiometry (oxides and sulphides). Techniques of introducing imperfections in solids. Electrical properties of solids: Conductivity of pure metals. Superconductivity. Photoconductivity. Photovoltaic effect. Dielectric properties. Piezoelectricity and ferroelectricity. Magnetic properties of solids: Diamagnetism, paramagnetism, ferromagnetism, ferrimagnetism and antiferromagnetism. Lasers and their applications.

Unit III Bioinorganic Chemistry

Metals in biological systems: Trace metals and ultratrace metals. The role of metal ions in biological systems. Biochemistry of iron: Iron storage and transport. Ferritin, haemosiderin and transferrin. Bacterial iron transport. Siderophores. Haemoglobin and myoglobin. Nature of haeme-dioxygen binding. Cooperativity in haemoglobin. Synthetic Blood. Cytochromes. Peroxydases and catalysases. Other natural oxygen carriers. Haemerythrins. Iron-sulphur proteins.

Unit IVOrganometallic Chemistry

Metal-metal bonds: Metal carbonyls, metal-carbonyl clusters, Bonding and structure Isoelectronic and isolobal relationships. Compounds with M-M multiple bonds. Quadrupole bonds. Relation of clusters to multiple bonds. One-dimensional solids.. Organometallic compounds: Preparation and general properties. Structure and bonding. Metal alkyls and aryls. Complexes with chain π-donor ligands: Allene, allyne, allyl and diene complexes. Hapto nomenclature. Complexes with cyclic π-donors: Cyclopentadiene, benzene, cycloheptatriene and cyclooctatetraene complexes. Oxidative addition and reductive elimination. Insertion and elimination.

References

1. F. A. Cotton and G. Wilkinson, “Advanced Inorganic Chemistry”, Wiley.
2. R. H. Crabtree, “The Organometallic Chemistry of Transition Metals”, 2Edn, Wiley.
3. V. Azaroff, "Introduction to Solids", McGraw Hill.
4. A. R. West, "Solid State Chemistry and its Applications", Wiley.
5. F. C. Phillips, “An Introduction to Crystallography”, Longman.

Further Reading

1. A. K. Galway, "Chemistry of Solids", Chapman Hall.
2. C. Kittel, “Introduction to Solid State Physics”, Wiley.

3. J. E. Huheey, “Inorganic Chemistry: Principles of Structure and reactivity”, Harper Collins.

CHE 532 ORGANIC SYNTHESIS AND BIOORGANIC CHEMISTRY 3 Credits

Unit I Organic Synthetic Strategies

Introduction to retrosynthetic analysis. Linear and convergent synthesis, Synthons, functional group equivalents and umpolung. Chemo, regio and stereoselectivity in synthesis. Protecting groups in organic synthesis, Baylis-Hilman, Sonogashira reaction. Glaser coupling, Shapiro, Peterson, Heck, Suzuki, Stille, McMurry, Wittig and related reactions. Functional group interconversions. Enol and enamine alkylation. Conversion of alkenes to diols. Organometallic [Mg, Cu Pd and Li] and organo-nonmetallic [Si, B, P and S] reagents in organic synthesis. Heterocyclic synthesis, nomenclature of heterocyclic compounds.

Unit II Reduction and Oxidation in Organic Synthesis

Catalytic hydrogenation and stereochemistry. Hydrogenation catalysts and their selectivity. Homogeneous hydrogenations. Fe, Zn, Na and Li reductions. Reduction using LAH, $NaBH_4$ and $NaCNBH_3$. Birch reduction. Lindlar catalysts and Rosenmund reduction. Clemmenson, Wolff Kishner and MPV reductions, hydrazine and diimide reductions. Oxidations using PCC, SeO_2, lead tetraacetate, ozone, HIO_4, OsO_4 and peracids. Dehydrogenation to aromatic compounds. Swern oxidation, Oppenauer oxidation. Sharpless asymmetric epoxidation, Woodward and Prevost hydroxylations

Unit III Natural Products Chemistry

Classes, typical examples and structures of secondary metabolites. Alkaloids, Terpenoids, Steroids and Prostaglandins, Chemical, spectroscopic and chiroptical methods for establishing carbon skeleton, functional groups and stereochemistry of natural products. Structure elucidation of santonin, reserpine, quercetin; β-carotene; ascorbic acid. Biosynthesis of terpenoids, fatty acids and polyketides, biosynthesis of papaverine

Unit IV Chemistry of Biopolymers and Polymers

Peptide bond formation methods, amino and carboxy protection in SPPS. Synthesis of A, G, C, T, U adenosine, ADP and ATP. Automated polypeptide and oligonucleotide synthesis. Structure organization of proteins and polynucleotides. Structure of polysaccharides including starch, cellulose, glycogen and chitin. Classes of polymers. Types and mechanisms of polymerization reactions. Methods of molecular mass and size distribution determination. Polymer structure and property characterisation. Synthesis of stereoregular polymers. Polymers in organic synthesis: supports, reagents and catalysts

References

1. S. Warren, “Organic Synthesis: The Disconnection Approach”, John Wiley, 2004.
2. W. Carruthers, “Some Modern Methods of Organic Synthesis”, Cambridge University Press, 2004.
3. J. R. Hanson, “Natural products: Secondary Metabolites”, RSC.
4. J. Mann and others,” Natural Products: Chemistry and Biological Significance", Longman.
5. F. W. Billmeyer, "Text Book of Polymer Science", Wiley.

Further Reading

1. R. K. Mackie, D. M. Smith and R. A. Aitken, “Guidebook to Organic Synthesis”, 3 Edn, Longman.
2. R. O. C. Norman and A. Coxon, "Modern Synthetic Reactions", Chapman Hall
3. H. O. House, "Modern Synthetic Reactions", Benjamin.
4. M. B. Smith, "Organic Synthesis", 2 Edn, McGraw Hill.
5. J. Mann, “Chemical Aspects of Biosynthesis”, Oxford primer 20, OUP.
6. R. J. Simmonds, "Chemistry of Biomolecules", RSC
7. R. H. Thomson, “The Chemistry of Natural products”, Blackie.

8. G. Odian, "Principles of Polymerization", Wiley.
9. R. J. Young, "Introduction to Polymer Science", Chapman Hall.
10. N. K. Krishnaswamy, "The Chemistry of Natural Products," Universities Press
11. S. V. Bhat, B. A. Nagasampagi and M. Sivakumar, "Chemistry of Natural products", Narosa, 2005
12. J. B. Harbourne, "Phytochemical Methods" Chapman Hall.

CHE 533 SURFACE CHEMISTRY, ELECTROCHEMISTRY and THERMODYNAMICS

3 Credits

Unit I Surface Chemistry

Types of surfaces. Thermodynamics of surfaces. Measurements of surface pressure and surface potential. Surfactants and miscelles. The gas-solid interface. Types of adsorption. Heat of adsorption. Adsorption isotherms. Gibb adsorption equation and its verification. Langmuir isotherm. Multilayer adsorption. Freundlich isotherm. BET isotherm. Solid-liquid interface. Influence of surface tension on adsorption. Measurements of surface area of solids. Harkin-Jure method. Entropy and point B methods. Use of Langmuir isotherm. BET method. Experimental methods for studying surfaces

Unit II Electrochemistry

Ionic activity. Ion-solvent interaction. Strong electrolytes. Ion transport. Debye-Huckel treatment. Onsagar equation. Debye-Falkenhagen effect. Wein effect. Types of electrodes. Electrochemical cells. Liquid junction potential. Evaluation of thermodynamics properties. Electrode-electrolyte interface. Electrokinetic phenomena. Current-potential curves. Over potential. Butler-Volmer equation. Tafel and Nernst equations. Corrosion and its control. Introduction to solid state electrochemistry.

Unit III Thermodynamics

First and second laws of thermodynamics. Thermodynamic criteria for equilibrium and spontaneity. The third law of thermodynamics. Need for the third law. Nernst heat theorem. Apparent exceptions to third law. Applications of third law. Thermodynamics of irreversible processes: Simple examples of irreversible processes. General theory of nonequilibrium processes. Entropy production. The phenomenological relations. Onsager reciprocal relations. Application to the theory of diffusion, thermal diffusion, thermoosmosis and thermomolecular pressure difference. Electrokinetic effects. The Glansdorf-Pregogine equation.

Unit IV Statistical Thermodynamics

Statistical thermodynamics: Mechanical description of molecular systems. Thermodynamic property and entropy. Microstates. Canonical and grand canonical ensembles. Equation of state for ideal quantum gases. Maxwell-Boltzman distribution. The partition functions. Partition function for free linear motion, for free motion in a shared space, for linear harmonic vibration. Complex partition functions and partition functions for particles in different force fields. Langevins partition function and its use for the determination of dipole moments. Electrostatic energies. Molecular partition functions. Translational, rotational, vibrational and electronic partition functions. Total partition functions. Partition functions and thermodynamic properties. Heat capacity of gases. Equipartition principle and quantum theory of heat capacity. Quantum statistics: Bose-Einstein statistics. Examples of particles. Theory of paramagnetism. Bose-Einstein condensation. Liquid helium. Super cooled liquid. Fermi-Dirac statistics. Thermionic emission. Relations between Maxwell-Boltzman, Bose-Einstein and Fermi-Dirac statistics. Heat capacity of solids. The vibrational properties of solids. Einstein theory of heat capacity. The spectrum of normal modes. The Debye theory. The electronic specific heat.

References

1. A. W. Adamson, "The Physics and Chemistry of Surfaces", Interscience.
2. S. J. Gregg, "The Surface Chemistry of Solids", Chapman Hall.
3. J. O. M. Bokris and A. K. N. Reddy, "Modern Electrochemistry", Wiley.
4. S. Glasston, "Introduction to Electrochemistry", East West Press Pvt Ltd. 1965.

5. E. N. Yenemin, "Fundamentals of Chemical Thermodynamics", MIR Publishers.
6. I.Prigoggine, “An Introduction to Thermodynamics of Irreversible Processes”, Interscience.

Further Reading

1. F. Daniels and R. A. Alberty, “Physical Chemistry”, Wiley.
2. W. D. Harkins, “The Physical Chemistry of Surface Films”, Reinhold.
3. D. R. Crow, “The Principle of Electrochemistry”, Chapman Hall.
4. F. W. Sears, “Introduction to Thermodynamics, Kinetic Theory of Gases and Statistical mechanics”, Addison Wesley.
5. P. W. Atkins, “Physical Chemistry”, OUP.
6. G. H. Maron and J. B. Land, “Fundamentals of Physical Chemistry”, Macmillan.

CHE 534 INORGANIC CHEMISTRY LAB-III 2 Credits

1. Analysis of fertilizers: Estimation of nitrogen in ammonium compounds. NPK estimations in synthetic fertilizers.
2. Analysis of some typical ores: Carbonate ore, sulfate ore, ilmenite and monazite.
3. Ion exchange separation of binary mixtures: Zn & Mg and Co & Ni.
4. Preparation and characterisation of complexes by UV-VIS, IR, magnetic susceptibility and electrical conductivity.

References

1. A. I. Weining and W. P. Schoder, "Technical Methods of Ore Analysis".
2. W. R. Schoder and A. R. Powell, "Analysis of Minerals and Ores of Rare Elements".
3. I. M. Kolthoff, V.J. Elving and Sandell, "Treatise on Analytical Chemistry", Interscience.
4. I. M. Kolthoff and Strenger, "Volumetric Analysis", Interscience.
5. Furman and Welcher, "Standard Methods of Inorganic Analysis", Van Nostrand.
6. W. G. Palmer, "Experimental Inorganic Chemistry", CUP.
7. R. S. Drago, "Physical Methods in Inorganic Chemistry", Affiliated East-West.

CHE 535 ORGANIC LAB-III 2 Credits

1. Estimation of esters, acids, reducing sugars, phenols, amines and ketones. [Assessement is based on % error]
2. Spectrophotometric estimation of cholesterol, ascorbic acid, glucose and ammonia. [Assessement is based on % error]

References

1. British Pharmacopoeia and Indian Pharmacopoeia.
2. A. C. Agarwala and R.M.Sharma, "A Laboratory Manual of Milk Inspection", Asia Publishing
3. V. K. Ahluwalia and R. Aggarwal, “ Comprehensive Practical Organic Chemistry” Vol 1 & 2, Universities Press.

CHE 536 PHYSICAL CHEMISTRY LAB-III 2 Credits

1. Conductance: Verification of Onsagar equation. Solubility of sparingly soluble substances. Oswald’s dilution law. Basicity of acids. Dissociation constants of acids and bases. Conductometric titrations involving acid-base and precipitation reactions. Equivalent conductance of solutions of strong electrolytes and weak electrolytes.

2. Potentiometry: Single electrode potentials of hydrogen and glass electrodes. Quinhydron electrode. Potentiometric titrations involving acid-base, redox and precipitation reactions. pH of buffer solutions. Solubility of AgCl. Determination of dissociation constant.
3. Polarography: Polarographic estimation of cadmium, zinc and lead. Composition of mixtures.
4. Flame photometry: Estimation of Na^+, K^+, Li^+, Ca^{2+} and Mg^{2+}. Composition of the mixtures.
5. Karl-Fischer titrator: Estimation of water contents in pharmaceuticals, oils, fats and paints.

References

1. J. B. Yadav, "Advanced Practical Chemistry", Goel Publishing House.
2. A. I. Vogel, "A Text Book of Quantitative Inorganic Analysis", Longman.
3. H. H. Willard, L. L. Merritt and J. A. Dean, "Instrumental Methods of Analysis", Affiliated East-West.

Elective courses:

CHE 501 ADVANCED INORGANIC CHEMISTRY 3 Credits

Unit I Inorganic Synthesis

Inorganic synthesis: Special techniques such as chemical vacuum line, plasmas, photochemical apparatus and electrolysis. Synthesis of the following non-metal compounds: BCl_3, AlF_3, SiF_4, NF_3, OF_2, S_2Cl_2, ClF_3, BrF_3, SbF_3, SbF_5, SF_4 and N_2F_4. Synthesis of transition metal complexes involving the following methods: Electron transfer reaction, substitution reaction, reactions of coordinated ligands, aldol condensation, imine bromination hydrolysis, substituent exchange reaction, template effect and macrocyclic ligands. Complexes with interlocking ring ligands. Formation of supramolecular species.

Unit II Bioinorganic Chemistry

Biochemistry of metals other than iron: Carboxypeptidase A, carbonic anhydrase and metallothioneins. Blue copper proteins Hemocyanins and oxydases Biomethylation of mercury. Nitrogenases. Molybdo-enzymes. Vanadium storage and transport. Alkali metals and regulation of membrane potentials. Ionophores. Ion pumps. Ca^{2+} in blood clotting. Mg^{2+} in phosphate transfer. Ru complexes. Nucleic acid structural probes. The application of therapeutic chelating agents and preformed coordination compounds.

Unit III Organometalic Chemistry

Anionic and hydrido clusters. LNCCs and HNCCs. Hetero atoms in metal clusters: Carbide and nitride containing clusters. Electron counting schemes for HNCCs. Capping rule. Chalcogenide clusters. Chevrel phases. Vibrational spectra of metal carbonyls. Carbonylate anions and metal carbonyl halides. Photochemical reactions of metal carbonyls. Nucleophilic and electrophilic attacks on CO. Metal nitrosyls and cyanides: Synthesis, structure and bonding. Metal isocyanides. Characterization of organometallic compounds. Fluxional molecules.

Unit IV Inorganic Photochemistry

Inorganic photochemistry: Photochemical laws and kinetics. Photophysical processes. Photo substitution, redox, dissociation and isomerization reactions. Photoreactions and solar energy conversions. Chlorophyll and photosynthesis. Photochemistry of photographic systems.

References

1. K. F. Purcell and J. C. Kotz, "Inorganic Chemistry", Saunders.
2. R. G. Wilkins, "Kinetics and Mechanism of Reactions of Transition Metal Complexes", 2Edn, VCH.
3. F. A. Cotton and G. Wilkinson, "Advanced Inorganic Chemistry", Wiley.
4. J. E. Huheey, "Inorganic Chemistry: Principles of Structure and Reactivity", Harper Collins.

5. J. A. Cowan, “Inorganic Biochemistry - An Introduction”, VCH.

Further Reading

1. I. Bertini, H. B. Gray, S. J. Lippard and J. S. Valentine, “Bioinorganic Chemistry”, Viva Books.
2. D. E. Fenton, “Biocoordination Chemistry”, Oxford Science.
3. W. W. Portfield, “Inorganic Chemistry - A Unified Approach”, 2 Edn. Academic.
4. V. Blazani and V. Carassiti, “Photochemistry of Coordination Compounds”, Academic.
5. A. W. Adamson and P. D. Fleischaner, “Concepts of Inorganic Photochemistry”, Wiley.

CHE 502 ADVANCED ORGANIC CHEMISTRY 3 Credits

Unit 1 Supramolecular Chemistry

The concept and development of supramolecular chemistry. Noncovalent interactions: Molecular and chiral recognition, Self-Assembly and Self-Organization, Molecular Aggregates: LB films, lipid membranes, nanotubes, miscelles and liquid crsytals, Host-Guest chemistry and inclusion complexes: crown ethers, cryptands, calixarenes, cyclophanes and cyclodextrins, Fullerene based supramolecular systems, Dendrimers, Molecular devices: molecular switches and wires,, Molecular recognition in bioprocesses. Codon and anticodon recognition. Protein biosynthesis, Introduction to DNA sequencing and PCR

Unit II Green Chemistry

Background, origin and principles of green chemistry. Atom economy and other metrics of greenness. Examples of green processes. Solid supports, Supercritical carbon dioxide, Microwave and sonochemical synthesis. Synthesis using solventless or alternate media conditions: fluorous and ionic liquid media. Green chemistry and sustainable development - pollution control to pollution prevention

Unit III Medicinal Chemistry and the Chemistry of the Cell

Introduction to drug discovery and design, drug administration, Drug action – pharmacokinetic and pharmacodynamic phases, Classification of drugs, Antibiotics and analgesics with examples. Drug stability, Biological membranes, Structure of biomembranes and their chemical models. Composition and structural features of lipids, Introduction to enzyme and coenzyme chemistry. Introduction to the chemistry of metabolism and metabolic cycles. Introductory bioenergetics

Unit IV Carbohydrate Chemistry

Carbohydrates: classification, configuration and conformation, Natural and synthetic monosacchardes, Chemical and physical properties, Oligo and polysaccharides, Carbohydrate containing molecules: Complex glycosides, Carbohydrate antibiotics, Nucleic acids, Glycoproteins, Peptidoglycans, Glycolipids, Chemical synthesis of oligosaccharides, Donor-acceptor concept, Anomeric effect, Preparation of glycosyl halides, Preparation of oligosaccharides by glycal method and n-pentenyl glycoside methods, Enzymatic and solid phase synthesis, Glycoconjugates: DNA binding of glycoconjudates,

References

1. J. M. Lehn, “Supramolecular Chemistry ”, VCH.
2. F. Vogtle, “ Supramolecular Chemistry ”, Wiley.
3. P. T. Anastas and J. C. Warner, “Green Chemistry: Theory and Practice,” OUP.
4. C. O. Wilson, O. Gisvold and R. F. Deorge “Text book of Organic, Medicinal and Pharmaceutical Chemistry”, J. B. Lippincott Company, Philadelphia (7^{th} Edn. 1977).
5. :Bioorganic Chemistry Carbohydrates” Edited by Sidney M Hecht, OUP, 1999.

Further Reading

1. J. W. Steed, and J. L. Atwood, Supramolecular Chemistry Wiley VCH, 2000
2. Helena Dodziuk, "Introduction to Supramolecular Chemistry" Springer, 2007.
3. Vincenzo Balzani, Alberto Credi and Margherita Venturi "Molecular Devices and Machines",: Wiley 2008.
4. Paola Ceroni, Alberto Credi and Margherita Venturi, 'Electrochemistry of Functional Supramolecular Systems', Wiley 2010.
5. A. Burger,"Medicinal Chemistry", Wiley Interscience, New York ((3rd Ed. 1970).
6. W. Kar, "Medicinal Chemistry ", Wiley Eastern.
7. A. Gringauz, "Introduction to Medicinal Chemistry", Wiley.
8. V. Kothekar, "Essentials of Drug Designing", Dhruv publications.
9. R. Sanghvi and M. M. Srivastava, "Green Chemistry", Narosa
10. P.S Kalsi and J. P Kalsi, "Bioorganic, bioinorganic and supramolecular chemistry" New age international, 2007.

CHE 503 ADVANCED PHYSICAL CHEMISTRY 3 Credits

Unit I Liquids, Emulsions and Liquid Crystals

X-ray diffraction study of simple liquids and their structures. Theories of liquid state. Oscillator. Free space and van der Waals theories. Lennard-Jones theory of melting. Specific heats of liquids.

Emulsions: macro- and micro-emulsions; aging and stabilization of emulsions; Phase behaviour of microemulsions.

Liquid crystals. Mesomorphic state. Types, examples and applications of liquid crystals. Theories of liquid crystals.

Unit II Industrial Catalysis and Femtochemistry

Metal complex catalyzed reactions. Hydrogenation. Wacker oxidation. Monsanto acetic acid synthesis. Hydroformylation. Thermal and photochemical Water Gas Shift reactions. Olefin metathesis. Fischer-Tropsch reaction. Mobil process for the conversion of methanol to gasoline hydrocarbons.

Ultrafast reaction dynamics. Introduction. Ultrafast lasers. Supersonic beams - pump-probe spectroscopy. Applications.

Unit III Phase Equilibria

Phase rule, Phase diagrams-binary, ternary, and metastable phase diagrams. Lever rule. Distillation of partially miscible liquids. Gibbs triangle. Inverse lever rule. Ternary isomorphous system. Law of adjoining phases. Boundary, boundary-curvature and solubility rules. Application in galvanizing. Thermodynamic calculation of phase diagrams. Microstructures. Analysis. Non-equilibrium microstructure. Effect of processing on microstructure. Second phase strengthening. Grain boundaries.

Unit IV Introduction to Computational Chemistry.

Empirical, Semi empirical and ab initio methods. Hartree-Fock SCF methods. Basis functions-STO and GTO. Basis sets. Minimal, split-valence, polarized and diffused. Molecular properties. Mulliken and natural charges. Dipole moments. Geometry. Molecular orbitals-occupied and virtual. Overlap and overlap population. Specification of molecular geometry in Cartesian coordinates and internal coordinates. Z-matrix of molecules H_2O, NH_3, CH_4, eclipsed and staggered ethane. Dummy atoms and ghost atoms.

References

1. L. C. Chapoy, "Recent Advances in Liquid Crystalline Polymers", Elsevier.
2. Bruce G Gates, "Catalytic Chemistry", John Wiley & Sons, Inc. USA, 1992
3. Femtochemistry: Ultrafast Dynamics of the Chemical Bond by Ahmed H. Zewail, 1994.
4. phase → P.W.Atkins, "Physical Chemistry", 2nd Edition, ELBS, 1985.

5. F.Daniels & R.A.Alberty, “Physical Chemistry”, 8th Edition, John Wiley.
6. G. K. Vemulapalli, Physical Chemistry, Printice Hall of India.
7. F. Jensen, “Introduction to Computational Chemistry”, 2nd Edition, Wiley, 1999.
8. C. J. Cramer, “Essentials of Computational Chemistry- Theories and Models”, Wiley, 2002.

SEMESTER IV

CHE 541 ANALYTICAL PRINCIPLES AND ENVIRONMENT 4 Credits

Unit I Analytical Principles-I

Accuracy and precision. The mean and median. Standard deviation, variance and coefficient of variation. Student “t” test. Confidence limits. Estimation of detection limits. Classification of errors. Distribution of random errors. Propagation of errors. Minimization of errors. Significant figures and computation rules. Approximation. Scatter diagram. Correlation coefficient, r. Calculation of r by the method of least squares. Correlation tables. Linear regression. Standard error of estimate. Nonlinear regression. Regression and ratio of variation.

Unit II Analytical Principles-II

Classification of reactions in volumetry (titrimetry). Acid-base equilibria in water. Ionization constant - role of solvent. Classification of solvents. Leveling and differentiating solvents. Acid-base equilibria in nonaqueous solvents. Buffers. Titration curves. Titrations in nonaqueous solvents. Theories of indicators of different types. Solubility products. Supersaturation and precipitate formation. Mechanism of precipitate formation. Aging of precipitates. Precipitation from homogeneous solutions. Purity of precipitate. Coprecipitation and postprecipitation. Contamination of precipitates. Washing of precipitate. Ignition of precipitate. Fractional precipitate. Organic reagents used in gravimetry - oxine, dimethylglyoxime and cupferron.

Unit III Environmental Chemistry-I

Scope of environmental chemistry. Environmental segments. Atmospheric composition. Atmospheric structure Heat balance of the earth. Chemical processes. Human activities and meteorology. Air pollutants Sulfur oxides Nitrogen oxides. Carbon monoxide. Cancer in our life style. Hydrocarbons as pollutants. Photochemical smog. Main components in photochemical smog. Green house effect. Consequences of Green house effect. Control and remedial measures of green house effect. Air pollution incidents. Acid rain. Control measures for air pollutants. Stratospheric chemistry-ozone. Antarctic and Arctic ‘ozone hole’ formation Abatement of ozone depletion. The Montreal Protocol.

Unit IV Environmental Chemistry-II

Water in the environment. Unique characteristics of water Pollution and environmental problems Waste disposal. Water pollutants. Organic matter in water. Oxygen demanding wastes. Soaps and detergents. Eutrophication. Oil pollution. Role of microorganism in oil cleanup operation. Heavy metals. Water treatment. Abatement procedures for water pollution.

Composition of lithosphere. Soil properties, pollutants in soil, nuclear waste disposal, radioactive pollutants, nuclear catastrophes, pollutants from industries and agriculture, future strategy for pesticide use, polymers and plastics, chemical toxicology, biochemical effects of pesticides and heavy metals, environmental management.

References

1. A. I. Vogel, " A Textbook of Quantitative Inorganic Analysis", Longman.
2. J. G. Dick, " Analytical Chemistry”, McGraw Hill.
3. D. A. Skoog, D. M. West and F. J. Holler, "Fundamentals of Analytical Chemistry", Saunders.
4. C. L. Wilson and D. W. Wilson, “Comprehensive Analytical Chemistry”, Vol. IB.

5. L. Meites, H. C. Thomas and R. P. Bauman, " Advanced Analytical Chemistry", McGraw Hill.

Further Reading

1. G. W. van Loon, “Environmental Chemistry”, OUP.
2. A. K. De, “Environmental Chemistry”, John Wiley.
3. G. S. Sodhi, “Fundamental Concepts of Environmental Chemistry”, Narosa.
4. K. B. Manjooran, “Modern Engineering Chemistry”, Kannatheri Publications, Kochi.
5. R. A. Bailey, H. M. Clark, J. P. Perris, S. Krause, R. L. Strong, “Chemistry of the Environment”Academic .

CHE 542 INSTRUMENTAL METHODS 4 Credits

Unit I Chromatographic Methods

Principles, instrumentation and applications of column chromatography, paper chromatography, thin layer chromatography, ion-exchange chromatography, gas chromatography and liquid chromatography. Hyphenated techniques, Analysis of samples using the above techniques.

Unit II Radiation Analysis Methods

Measurement of radioactivity. Detection counters. ionization chamber, cloud chamber, Bubble chamber, proportional counter, the Geiger counter, scintillation counters, Neutron activation analysis. Isotope dilution methods. Working of nuclear reactors.

Unit III Electroanalytical Methods

Principles, instrumentation and applications of electrogravimetry, coulometry, polarography, amperometry, cyclic voltametry, potentiometry and conductometry. Analysis of samples using the above instruments.

Unit IV Thermal and Surface Analysis Methods

Principles, instrumentation and applications of thermogravimetry (TG), derivative thermogravimetry (DTG), differential thermal analysis (DTA) and differential scanning calorimetry (DSC). Analysis of samples using the above instruments, Introduction to AAS, SEM, TEM, AFM and other surface characterization techniques.

References

1. A. I. Vogel, “A Textbook of quantitative Inorganic Analysis”, Longman.
2. D. A. Skoog, D. M. West and F. J. Holler, "Fundamentals of Analytical Chemistry", Saunders
3. F. A. Settle (Ed.), “Handbook of Instrumental Techniques for Analytical Chemistry”, Pearson
4. R. S. Drago, "Physical Methods in Inorganic Chemistry", Affiliated East West .
5. L. L Willard, H. H. Merit and J. A. Dean, "Instrumental Methods of Analysis", Affiliated East-West
6. W. W. Wendlandt, “Thermal Analysis”, 3 Edn., Wiley.
7. T. Hatakeyama and F. X. Quinn, “Thermal Analysis”, Wiley

CHE 543 Dissertation 6 Credits

Each student must carry out an original research in a topic in accordance with the electives chosen during Semesters III and IV and under the guidance and supervision of a faculty member of the Department as the course advisor.

Elective courses:

CHE 504 APPLIED CHEMISTRY 4 Credits

Unit I Petroleum, Fuels & Combustion, Lubricants

Petroleum: Petroleum, cracking, Synthetic petrol, Refining of gasoline, Reforming, Chemical structure of fuel and knocking. Octane Rating of fuels, Cetane Rating, Diesel engine fuel, Kerosene, LPG as a fuel.

Fuels & Combustion: Classification, Calorific value, Types, Determination by Bomb calorimeter, Dulong's Formula, Analysis of Coal, Proximate and Ultimate analysis, Fuel gas analysis, Significance, Numericals, Carbonization of Coal, Manufacture of metallurgical coke by Otto Hoffman's byproduct oven, Combustion calculations.

Lubricants: Functions of' lubricant, Mechanism of lubrication, Fluid or Hydrodynamic Lubrication, Thin film or Boundary lubrication & Extreme pressure lubrication. Lubricants for Extreme ambient conditions and for special applications. Properties of lubricants and tests.

Unit II Corrosion and Protective Coatings

Corrosion and its Control: Nernst Theory, Standard Electrode Potential, Galvanic Series, Concentration cell, Types of corrosion: Uniform and Galvanic, Erosion, Crevice, Pitting, Exfoliation and Selective leaching, Inter-angular Stress, Waterline, Soil, Microbiological. Theories of corrosion: Acid, Direct Chemical attack, Electrochemical, Corrosion reactions, Factors affecting corrosion, Protective measures against corrosion, Sacrificial anode, and impressed current cathode protection.

Protective Coatings: Paints: Constituents, functions & mechanism of drying. Varnishes and Lacquers; surface preparation for metallic coatings, electroplating (gold) and electrode less plating (Nickel), anodizing, phosphate coating, powder coating & antifouling coating.

Unit III Applied Inorganic Chemistry

Introduction to chemical industry: Flow sheet preparation. Principles of process selection and operation selection. Basic raw materials and routes to major inorganic products. Flow sheets and engineering aspects of the manufacture of sulfuric acid, ammonia, urea, glass.

Portland Cement: Manufacture of cement, Dry and Wet process, Flow sheet and engineering aspect of the manufacture of Portland cement, Important process parameters for manufacturing a good cement clinker. Characteristics of the constitutional compounds of cement.

Additives for cement, Properties, General composition, testing of cement, Chemical & physical requirement.

Refractories: Definition, Classification with Examples; Criteria of a Good Refractory Material; Causes for the failure of a Refractory Material. Flow sheet and engineering aspect of the manufacture of Refractories.

Unit IV Applied Organic Chemistry

Raw materials and routes to major organic products. Flow sheets and engineering aspects of the manufacture of important products such as nitrobenzene, vinyl chloride, soaps, detergents and hydrogenation of oils.

Pharmaceuticals: manufacturing process of aspirin, vitamin A and paracetamol.

Pesticides: manufacture of BHC, DDT, Carbaryl and Malathion. Manufacture of dyes.

Cosmetics: Talcum Powder, Tooth pastes, Shampoos, Nail Polish, Perfumes, soaps, and detergents - General formulations and preparation - possible hazards of cosmetics use.

Adulterants: Adulterants in milk, ghee, oil, coffee powder, tea, asafoetida, chilli powder, pulses and turmeric powder - identification.

Color chemicals used in food-soft drinks and its health hazards

Polymers: Types of Polymerization. Thermoplastics & thermosetting polymers. Preparation, properties and applications of the Polyethylene, Teflon, PVC, Nylon, Phenol formaldehyde & Urea Formaldehyde. Silicone resins, silicone fluids, silicone greases. Polyurethanes, foamed or cellular plastics. Elastomers: Natural rubber, Vulcanization of rubber & Synthetic rubber.

References

1. Muncipal water and waste water treatment-Rakesh kumar & R N Singh, Teri Press, 2008
2. Environmental Management-Vijay Kulkarni & T V Ramachandran, Teri Press, New Delhi, 2009.
3. Water pollution and management - C.K. Varashney - Wiley Eastern Ltd., Chennai - 20.
4. Industrial Solid Wastes-A.D Patwardhan, Teri Press New Delhi, 2012
5. Environmental Chemistry-Collin Baird, Publisher WH Freeman, 2008

Further Reading

1. Chemical process industries - Shreve R. Norris & Joseph A.Brink.Jr, McGraw Hill, 1984.
2. Perfumes, Cosmetics and soaps - W.A. Poucher (Vol 3), Springer, 2000.
3. Environmental Chemistry - A .K. DE
4. Industrial Chemistry, B.K. Sharma- Goel publishing house, Meerut.
5. Food Science - III Edition - B. Srilakshmi - New age international publishers 2005.
6. Food chemistry Lillian Hoagland Meyer - CBS publishes & distributors - 2004.
7. Fundamental concepts of applied chemistry - Jayashree Ghosh - S.Chand & Co Ltd., New Delhi.
8. Applied chemistry - K.Bagavathi Sundari - MJP Publishers
9. P.Wiseman, "Industrial Organic Chemistry". Elsevier Science Ltd, 1972.
10. Charles E.Dridens, "Outline of Chemical Technology". East-West Press Publishing, 1973

CHE505 APPLIED ELECTROCHEMISTRY 4 Credits

Unit I Electrochemical Techniques

Current and Potential: i-E relation; Basics of electrodes and electro-sensing, Polarisation of electrodes, Cyclic voltametry - analysis of voltamograms, Linear sweep voltametry-, Potential step method; Chrono amperometry- Ilkovic equation, Electrochemical Impedance Spectroscopy: derivation of kinetic parameters, Analysis of Nyquist and Bode plots of simple redox reactions, Electrocatalysis:, Electrochemical catalysts with special reference to oxides and mixed oxides of d and f block elements. Electronic and geometric factors in electrocatalysis. Mechanism of hydrogen evolution reactions.

Unit II Energy Storage Systems

Electrochemical storage cells: Charging and discharging, storage density, energy density. Different types of batteries: (i) Lead Acid (ii) Nickel-Cadmium, (iii) Zinc manganese dioxide. Modern batteries: (i) Zinc-Air (ii) Nickel-Metal Hydride, (iii) Lithium battery. Fuel cells; thermodynamic efficiency, electromotive force of fuel cells: Low temperature fuel cells: Hydrogen–oxygen fuel cells–alkaline and polymeric membrane types. Basics of Microbial fuel cells: construction, electrodes used, electron transfer mechanism.

Unit III Corrosion and Management

Classification of corrosion, Mechanism of corrosion of metals, thermodynamics of corrosion–Pourbaix diagrams. Passivation-definition and anodic passivation theory. Corrosion current and corrosion potential- Evan's diagrams. Types of prevention methods: Modification of the substrate, Modification of the environments: inhibitors, Control of interface: cathodic and anodic protection in detail.

Unit IV Industrial Metal Finishing

Metal finishing techniques: Electroplating- faradays laws, current efficiency, throwing power, alloy plating, composite plating. Eletcroless nickel plating: Fundamental aspects, bath components, reducing agents complexing agents, stabilizers, effect of temperature and pH of the bath. Properties and applications of electroless nickel plating. Galvanic coatings: Hot dip zinc coatings – principles, surface preparation, methods, applications.

References

1. James A. Plam Beck, "Electroanalytical Chemistry- Basic Principles and Applications", John Wiley & sons, Wiley Publication, 1982.
2. B.H. Vassos and G.W. Ewing, "Electroanalytical Chemistry", John Wiley & Sons, 1983.
3. M. E. Oraze, B. Ttribolletm " Electrochemical Impedance Spectroscopy" John Wiley & Sons, 2008.
4. J.O.M. Bockris & A.K.N. Reddy, "Modern Electrochemistry", Plenum Press, Vol–II, 1996.
5. A.J. Bard & L.R. Faulkner, "Electrochemical Methods Fundamentals and Applications", John Wiley & Sons. 2nd Edition, 2001.
6. J.O.M. Bockris & A.K.N. Reddy, "Modern Electrochemistry 2B: Electrodes in Chemistry, Engineering, Biology and Environmental Science", Vol–II, Springer 81, 2001.
7. R. Narayanan and B. Viswanathan, Chemical and Electrochemical Energy Systems, Orient Longmans, 1997.
8. A. S. J. Appleby and F. K. Foulkes, Fuel cell Hand Book, Von Nostrand Reinhold, 1989.
9. D. Linden, Hand book of batteries and Fuel cells, McGraw Hill Book Company, 1984.
10. O' Hayre, Ryan, Suk-Won Cha, Whitney Colella, and Fritz B. Prinz. Fuel Cell Fundamentals. 2nd ed. John Wiley & Sons, 2009.
11. L.L. Shreir, Corrosion, Vol I and Vol II, Newness Butterworths, Edward Arnold Ltd, London.
12. S.N. Banerjee, "An Introduction to Corrosion Science and Corrosion Inhibition", Oxonian Press P. Ltd., New Delhi, 1985.
13. V.S. Sastry, "Corrosion Inhibitors, Principles & Applications", V.S. Sastry, John Wiley & Sons.
14. G.O. Mallory, J.B. Hajdu, "Electroless Plating-Fundamentals and Applications", American Electroplaters and Surface Finishers Society, 1990.
15. F.A.Lowenheim, "Modern Electroplating", John Wiley and Sons INC. USA, 3rd Edition, 1974.
16. R.F.Bunshah, "Handbook of deposition technologies for films and coatings, science, technology and applications", Noyes publications, New York, 1994.

CHE 506 CHEMISTRY OF NANOMATERIALS 4 Credits

Unit 1 Properties of Nanomaterials

Difference in behavior between bulk and nanomaterial's, Size and dimensionality effects, Quantum size effect. Nanoscale confinement of electronic interactions, Quantum confined materials, Novel optical and magnetic properties of nanomaterials. Quantum dots and its fluorescence, Up conversion and down conversion, Metal nanoparticles, Surface Plasmon Resonance, Magnetic nanoparticles, Superparamagnetism in nanoparticles. Environmental Issues of nanomaterials

Unit II Chemical Interaction at Nanoscale

Interparticle interactions in nanoscale, Types of intermolecular bonding, Electrostatic interactions,- Ionpair intractions, solvent effects, ion dipole and dipole dipole interactions, Dative bond, π interactions hydrogen bonding, Vander waals attractions and its physical property dependence, hydrophobic effect, Ostwald ripening. Reverse micelle as Spherical nanoreactors.

Unit III Nanostructured Molecular Architectures.

Carbon fullerenes, its structure and applications, Superconductivity in C_{60}. Carbon nanotubes, its structure electrical and mechanical properties and its applications. Semiconductor nanomaterials, Graphenes, Carbon dots, Dendrimers. Biological nanomaterials, biomimetics, Self assembly of proteins, micelles and vesicles. Liposomes Core shell structures, Ferrofluids.

Unit IV Synthesis, Characterization and Applications of Nanomaterials

Solution based synthesis of nano particles , Synthesis of quantum dots, silver and gold nanoparticles using aqueous chemical method, Brief introduction to vapour phase synthesis of nanoparticles. Synthesis using frame work, support and substrates, Introduction to Physical vapour deposition, Molecular beam epitaxy, Chemical vapour deposition, Chemical beam Epitaxy, LAVD, Atomic layer deposition, Electrospinning and Lithographic techniques

Optical Characterization, UV Visible Spectroscopy, Spectrofluorometry, Dynamic light scattering method, Surface Plasmon resonance spectroscopy. Structural Characterization. Using AFM,STM, SEM, HRTEM ,SERS

Nanophotonic devices, Nanophotonics for biotechnology and nanomedicine Magnetic nanoparicles as MRI Contrast agents, Drug delivery, Nanoparticle for optical diagnosis and targeted therapy, Bio-imaging with quantum dots, FRET, Nanosensors,

References

1, G. L. Hornyak, Harry F. Tibbals, Joydeep Dutta, John J. Moore, Introduction to Nanoscience and nanotechnology, CRC Press, London 2009.

2, Paras M Prasad - Nanophotonics.John Wiley and Sons,New Jersey,2004

3, Geoffrey A. Ozin & Andre C. Arsenault , Nanochemistry, A chemical approach to nonmaterial's; RSC Publishing 2005

4, Charles P. Poole Jr & Frank J Owens; Introduction to Nanotechnology, Wiley, India , 2008

5, Richard Booker, Earl Boysen, Nanotechnology, Wiley, India 2005.

6, Pradeep T. Nano the essentials, Understanding Nanoscience and Technology, McGraw – Hill Education, NewDelhi 2007.

CHE 507 ELECTRONIC STRUCTURE THEORY AND APPLICATIONS 4 Credits

Unit I Empirical and Semi-Empirical Methods

Brief description of computational methods: *ab initio*, semi empirical, and empirical methods. Molecular mechanics. Potential energy functions. Force fields. Geometry minimization, Molecular dynamics. Harmonic oscillator trajectories. Introduction to stochastic dynamics, Monte Carlo simulations. Simulation convergence. Extended Hückel theory. Introduction to CNDO, INDO, NDDO.

Unit II *Ab initio* Methods and Polyatomic Calculations

Roothaan Hartree Fock method. Self consistent field. Slater determinants. Computing the matrix elements. Slater's rules for matrix elements. Convergence. Optimization. Basis functions. STO and GTO. Basis sets. Contracted and primitive. Minimal, split-valence, polarized and diffused. Effective core potential, ECP. SCF orbital energies. Koopmann's theorem and Brillouin theorem. Examples of closed and open shell calculations. Influence of point group in computations. Illustration by taking H_2O, and NH_3. Computing the quantities- structure, potential energy surface, and chemical properties such as Mulliken and natural charges. Dipole moments. Avoided crossings and configuration mixing. Exchange and Correlation energy. Configuration Interaction (CI). Moller-Plesset Perturbation Theory (MP_n).

Unit III Density Functional Theory

Development of density function theory (DFT). Density matrices. Thomas-Fermis model. Hohenberg-Kohn existence and variational theorems. Chemical potential. Kohn-Sham self consistent field method. Exchange correlation functionals. Local density approximation (LDA), density Gradient corrections (GGA). Hybrid and meta –GGA functionals. Advantages and applications of DFT.

Unit IV Applications

Specifying the molecule in Cartesian and internal coordinates: Writing the Z-matrix of H_2O, CH_4, ethane, Cyclopentadiene, and benzene with suitable point group.

Lab:

1. Semi-empirical calculation-1: Optimize the geometry of H_2O, CH_4, ethane, Cyclopentadiene, and benzene using MOPAC and compute the single point and optimized energies.
2. Semi-empirical calculation-2: Constructing the correlation diagram using EH method for a) Diels-Alder reaction between ethylene and butadiene. b) dimerization reaction between two ethylenes. Analyze the results.
3. *Ab initio* calculation - Optimize the structures from 1 using NWChem software at HF and DFT level. Correlate the results.

References

1. F. Jensen, "Introduction to Computational Chemistry", 2nd Edition, Wiley, 1999.
2. D. Young "Computational Chemistry – A Practical Guide", Wiley, 2001.
3. C. J. Cramer, "Essentials of Computational Chemistry- Theories and Models", Wiley, 2002.
4. A. R. Leach, "Molecular Modeling – Principles and Applications, Addison Wesley Longman, 2001
5. J. Foresman and A. Frisch " Exploring chemistry with electronic structure methods", Guassian Inc, 2000.
6. I. N. Levine, "Quantum Chemistry", 6th Edition, Pearson Education Inc., 2009.
7. D. A. McQuarrie, "Quantum Chemistry", University Science Books, 1983.

CHE 508 PHOTOPHYSICAL PROCESSES AND APPLICATIONS 4 Credits

Unit I Photophysical Properties of the Electronically Excited Molecules

Basic principles of photochemistry: Absorption of radiation-Beer Lambert's law. Electronic transitions. Frank Condon principle. Jablonski diagrams. Nonradiative transitions. Internal conversion and inter system crossing. Radiative transitions: Fluorescence emission, triplet states and phosphorescence. Absorption complexes. Charge transfer absorption. Excimers. Exciplexes. Delayed fluorescence. Chemiluminescence.

Unit II Bimolecular Processes

Fluorescence quenching. Collisional quenching. Stern-Volmer equation. Static quenching Photoinduced electron transfer (PET): Concepts and theories, electron donors and acceptors, quantum yield, efficiencies and lifetimes, intermolecular, intramolecular and supramolecular PET. Fluorescence resonance energy transfer (FRET): Trivial or radiative mechanism; Forster and Dexter type energy transfer. Energy transfer versus electron transfer.

Unit III Techniques and Instrumentation

UV-Vis spectrophotometry. Steady-state fluorescence spectroscopy. Lasers as excitation sources, Time-resolved fluorescence spectroscopy, Detection and kinetics of reactive intermediates. Transient absorption spectroscopy.

Unit IV Solar Energy Conversion

Natural photosynthetic system. Conversion of solar energy to chemical and other forms of energies. Solar water splitting. Photocatalytic carbon dioxide reduction. Photovoltaic cells: Polymer solar cells and dye sensitized solar cells. Photo-biochemical energy production

References

1. K. K. Rohatgi-Mukherjee, "Fundamental of Photochemistry", New Age International (P) Ltd., New Delhi, 1986.
2. J. R. Lakowicz, "Principles of Fluorescence Spectroscopy", 3rd Ed., Springer, New York, 2006.
3. G. J. Kavarnos, "Fundamentals of Photoinduced Electron Transfer", VCH publishers Inc., New York, 1993.

4. N. J. Turro, V. Ramamurthy, J. C. Scaiano, “Principles of Molecular Photochemistry”, University Science, Books, CA, 2009.
5. C. H. Depuy and O. L. Chapman, “Molecular Reactions and Photochemistry”, Prentice Hall of India Pvt. Ltd., 1988.
6. B. Valeur, “Molecular Fluorescence: Principles and Applications,” Wiley-VCH Verlag GmbH, Weinheim, 2002.
7. M. Gratzel, “Energy Resources through photochemistry and catalysis,” Academic Press, 1983.
8. N. Serpone and E. Pelizzetti, “Photocatalysis,” Wiley, New York,1989.

CHE 509 ORGANIC SYNTHESIS 4 Credits

Unit I The Disconnection Approach

Designing a synthesis, FGI, Synthons, order of events, choocing a disconnection, synthesis of aromatic compounds, chemoselectivity in synthesis – one group C-X disconnections – alcohols, ethers, sulphides, alkyl halides, two group C-X disconnections,1,1 and 1,2-C-C disconnections one group C-C disconnections, enolate chemistry, two-group disconnections, 1,1-,1,2-- 1,3-, 1,4- and 1,5-difunctionalized compounds

Unit II Retrosynthesis in Action

Advanced strategies, retrosynthesis in industry, stereoselectivity and regioselectivity in synthesis, using alkenes, alkynes and nitro compounds in synthesis, reconnections, retrosynthetic analysis and synthesis – practice problems

Unit III Heterocyclic Ring Synthesis

Three, four five and six membered ring synthesis and retrosynthesis, aromatic heterocycles, aromatic heterocylces with two heteroatoms, rearrangements in synthesis, electrophilic substitution reactions, named reactions in heterocyclic synthesis

Unit IV Modern Organic Synthesis

Organocatalysis, NHC;s – synthesis and reactivity, Transition metal mediated reactions in organic synthesis, Olefin metathesis, Grubbs catalysts, enzymes in organic synthesis, Palladium mediated coupling reactions, Total synthesis of certain natural products – tetrodotoxin, strychnine, tetracycline, sordaricin, ingenol.

References

1. Organic Synthesis – The disconnection approach” Stuart WarrenJohn Wiley and Sons, 2004
2. “Organic Chemistry” Clayden, Greeves, Warren and Wothers, Oxford University press, 2001
3. T. L. Gilchrist, “Heterocyclic Chemistry.” Pearson, Third Edn., 2005
4. Joule J. A and Mills, K. Heterocyclic Chemistry, 4th Edition, UK, Blackwell Science, 2000
5. **“**Oeganic Synthesis – state of the art 2003-2005”. Douglas Taber

Further Reading

1. R. O. C. Norman, “Principles of Organic Synthesis”, Chapman and Hall 2nd Edition, 1995.
2. Organic Chemistry” Clayden, Greeves, Warren and Wothers, Oxford University press, 2001
3. Francis A.Carey and Richard J. Sundberg, “Advanced Organic Chemistry - Part B: Reactions and Synthesis”, 5th Edition, Springer, 2007.

CHE 51B ANALYTICAL AND ENVIRONMENTAL CHEMISTRY 2 Credits

Unit I Data Analysis

Accuracy and precision. Evaluation of analytical data, The mean and median. Standard deviation, variance and coefficient of variation. Classification of errors. Minimization of errors. Significant figures and computations. Statistical methods in analysis. Students T test, Rejection of suspected value, Q test

Unit II Volumetric analysis and precipitation methods

Classification of reactions in volumetry (titrimetry). Acid-base equilibria in water. Buffers. Titration curves. Theories of indicators. Theory of complexometric titrations and applications, Solubility product. Common ion effect. Super saturation and precipitate formation. Precipitation from homogeneous solutions. The purity of precipitate. Coprecipitation and postprecipitation. Contamination of precipitates. Washing of precipitate. Ignition of precipitate. Organic reagents used in gravimetry.

Unit III Introduction to Environmental Chemistry-

Components of Environment. Environment and development. Earth's atmosphere, Stratosphere chemistry, Processes for catalytic decomposition for ozone, Chlorofluorocarbons, Protection of ozone layer, Chemistry of photochemical smog, Composition of rain, Atmospheric production of nitric Acid, sulphuric acid, Rain, snow and fog chemistry, Aerosols, Adverse effects of acid rain, Green house effect. Impact of green house effect on global climate. Air pollution incidents. Control measures for air pollution.

Unit IV Hydrosphere and solid waste management

Physical and chemical properties of water, Organic matter in water, Humic material, Metal complexes of ligands of anthropogenic origin, Water pollutants,. Soaps and detergents. Eutrophication. Oil pollution. Heavy metals. Industrial waste water treatment: Solid wastes from mining and metal production, Organic wastes, Mixed urban wastes, Solid waste management, Pollutants in soil. Radioactive pollutants. Pollutants from industries and agriculture. Chemical toxicology. Biochemical effects of pesticides and heavy metals.

References

1. A. I. Vogel, " A Textbook of Quantitative Inorganic Analysis", Longman.
2. D. A. Skoog, D. M. West and F. J. Holler, "Fundamentals of Analytical Chemistry", Saunders
3. C. L. Wilson and D. W. Wilson, "Comprehensive Analytical Chemistry", Vol. IB.
4. G. W. van Loon, "Environmental Chemistry", OUP.
5. A. K. De, "Environmental Chemistry", Wiley Eastern.
6. G. S. Sodhi, "Fundamental Concepts of Environmental Chemistry", Narosa.
7. K. B. Manjooran, "Modern Engineering Chemistry", Kannatheri Publications, Kochi.
8. R. A. Bailey, H. M. Clark, J. P. Perris, S. Krause and R. L. Strong, "Chemistry of the Environment", Academic.