COCHIN UNIVERSITY OF SCIENCE AND TECHNOLOGY

DEPARTMENT OF APPLIED CHEMISTRY

SYLLABUS FOR M.Sc. APPLIED CHEMISTRY

(*WITH EFFECT FROM 2013-14*)

CORE

CHE 2101 Inorganic Chemistry-I

(3 Credit) **48 Hours**

Unit 1

Structure and bonding in polyhedral boranes and carboranes, styx notation; electron count in polyhedral boranes;Wade's rule; topological approach to boron hydride structure. Styx numbers. Importance of icosahedral framework of boron atoms in boron chemistry. Closo, nido and arachno structures. synthesis of polyhedral boranes; Carboranes Metallocarboranes. boron halides; phosphine-boranes; boron heterocycles; borazine.

Unit 2

Sulphur-Nitrogen compounds: Tetrasulphur tetranitride, disulphur dinitride and polythiazyl. S_xN_y compounds. S-N cations and anions. Sulphur-phosphorus compounds: Molecular sulphides such as P_4S_3, P_4S_7, P_4S_9 and P_4S_{10}. Phosphorus-nitrogen compounds: Phosphazenes. Cyclo and linear phosphazenes.

Unit 3

Silanes, silicon halides, silicates, silicones, silanols; germanium, tin and lead organyls; silenes, germenes and stannenes; fullerenes; carbon nanotubes (CNT's) and graphenes ultramarines and zeolites

Unit 4

Relative strength of acids, Pauling rules, Lux-Flood concept, Lewis concept, Measurement of acid base strength sytematics of Lewis acid –base interactions steric and salvation effects acid –base anomalies , Pearson's HSAB concept, acid-base strength and hardness and softness, Symbiosis, theoretical basis of hardness and softness, electronegativity and hardness.

Chemistry in non aqueous solvents reactions in NH_3, liquid SO_2, solvent character, reactions in SO_2, acetic acid, solvent character, reactions in CH_3COOH and some other solvents. Molten salts as non aqueous solvents solvent properties room temperature molten salts. unreactivity of molten salts, solutions of metals.

Unit 5

Macrocycles and supramolecules non-covalent forces and interactions in supramolecules,:crown ethers, cryptates, cryptands,carcerands, calixarenes, cyclodextrins, fullerenes, dendrimers, rotaxanes, cucurbiturils, self-assembly and preorganization, coordination driven self-assembly of supramolecular two and three dimensional architectures, host-guest chemistry, metal-organic frameworks and their applications,

References:

1. F. A. Cotton, G. Wilkinson, C. A, Murillo, and M. Bochmann Advanced Inorganic Chemistry, 6th Edition Wiley-Interscience: New York, 1999.
2. J.E. Huheey, Ellen A. Keiter and Richard L. Keiter "Inorganic Chemistry, Principles of structure and Reactivity", 4th Ed., Harper Collin College Publishers, 1993
3. J. W. Steed, J. L. Atwood, Supramolecular Chemistry, 2nd edition, John Wiley & Sons Ltd., (2009)
4. D. F. Shriver, P. W. Atkins, C. H. Langford, Inorganic Chemistry, 3rd Ed. ELBS, 1999.
5. B. Douglas, D. McDaniel, J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Ed., Wiley.
6. N. N. Greenwood, A. Earnshaw, Chemistry of the Elements, 2nd Edn., BH, 1997.

CORE

CHE 2102 Organic Chemistry I

(*Structure, Reactivity, Reactions and Mechanisms*)

(3 Credit) **48 Hours**

Unit 1 (8 hours)

Structure and Models of bonding: Study of different bonding models with emphasis on understanding three dimensional structure of molecules. Bonding weaker than covalent bonds: ion pairing interactions: ion - dipole interactions, dipole - dipole interactions, hydrogen bonding, factors affecting the strength of hydrogen bonds, cation-pi interaction, polar-pi interaction, pi stacking, pi donor-acceptor interactions. Hydrophobic effect, Concept of supramolecular chemistry.

Unit 2 (10 hours)

MOT and structures of organic molecules: Qualitative MOT. Group Orbitals of Methyl and Methylene groups. MO's of Methane, ethane, propane, methyl halides, ethylene, formaldehyde, conjugated systems: 1,3-butadiene, allyl radical and anion. Structure and stability of reactive intermediates: carbocations, carbanions, radicals, carbenes and nitrenes (excluding reactions and synthetic applications). Effects of pi conjugation, alkene, anion, cation and radical stabilizing groups, hyperconjugation, effects of hyperconjugation with C-H bonds, C=C, lone pairs, cations, negative hyperconjugation, anomeric effect. Huckel's rule and modern theory of aromaticity. Study of [n]annulenes, fullerenes, nonbenzenoid aromatics. Frontier Orbitals, HSAB concept, Perturbation theory of reactivity.

Unit 3 (10 hours)

Classification of reactions according to IUPAC conventions. Reaction mechanism-guidelines on Pushing of electrons, methods of determining reaction mechanisms (kinetic and non kinetic methods). The Hammond postulate, reactivity vs selectivity principle, the Curtin-Hammett principle, microscopic reversibility, kinetic vs thermodynamic control. Isotope effects, Effect of structure on acidity and basicity. Linear free energy relationships: Hammett and Taft parameters, Solvent effects (Grunwald-Winstein plots and Schleyer adaptation), nucleophilicity and nucleofugality. Other Experimental techniques to determine reaction mechanisms: identification of intermediates by trapping and competition experiments, cross - over experiments, isotope scrambling, radical clocks and traps, matrix isolation. Baldwin ring-closure rules.

Unit 4 (12 Hours)

Substitutions on aliphatic carbons (saturated and unsaturated): Mechanism of Nucleophilc, Electrophilic and free radical substitutions. Application of Frontier Orbital theory in studying ionic reactions: aliphatic nucleophilic substitution reactions, Ambident nucleophiles, Ambident electrophiles, α-effect. Application of Frontier Orbital theory in studying radical reactions. Mechanisms of polar and nonpolar additions and eliminations (excluding pericyclic reactions).

Unit 5 (8 Hours)

Substitutions on aromatic carbon: Mechanism of electrophilic, nucleophilic and free radical substitutions. Application of Frontier Orbital theory in studying aromatic substitution reactions.

References:

1. J. March: Advanced organic chemistry-reactions mechanisms and structure, 4th Ed., John Wiley.
2. E. V. Anslyn and D. A. Dougherty: Modern Physical Organic Chemistry. University Science Books, 2006 edition.
3. F. A. Carroll: Perspectives on structure and mechanism in organic chemistry, Wiley.
4. T. H. Lowry and K. S. Richardson: Mechanism and Theory in Organic Chemistry, 3rd Ed., Addison-Wesley.
5. F. A. Carey and R. J. Sundberg: Advanced Organic Chemistry Parts A and B, Fifth Edition, Springer.
6. N. S. Issacs: Physical Organic Chemistry, Second Edition, John Wiley and Sons.
7. A. Pross: Theoretical and Physical Principles of Organic Chemistry, John Wiley.
8. J. Clayden, N. Green, S. Warren and P. Wothers: Organic Chemistry, Oxford University Press.
9. S. H. Pine: Organic Chemistry McGraw Hill.
10. I. Flemming: Frontier Molecular Orbitals in Organic Chemistry, John Wiley.
11. I. Flemming: Molecular orbitals and organic chemical reactions, student edition, Wiley.
12. J. McMurry, Organic Chemistry (Fifth Edition), Brroks/Cole .
13. R. Bruckner, Advanced organic chemistry: Reaction Mechanisms. Academic Press.

CORE

CHE 2103 Physical Chemistry I

(3 Credit) **48 Hours**

Unit 1 Quantum Chemistry 1

Postulates of Quantum Mechanics. Time dependent and time independent Schrodinger wave equation. Conservative systems, Stationary states, Formulation of quantum mechanical problems, Application of Schrodinger wave equation for particle in one dimensional box, Particle in three dimensional box (rectangular and cubical), Separation of variables, concept of degeneracy, Introduction to quantum mechanical tunneling

Unit 2 Quantum Chemistry 2

Vibrational motion, Harmonic oscillator, Method of power series, Hermite equation and Hermite Polynomials, Recursion formula, Rodrigues formula, wave function and energy . Rigid rotator, Wave function in spherical polar coordinates, Planar rotator, phi equation, wave functions in real forms, Polar diagrams, Nonplanar rotator, Theta equation and solutions Lagendre equation and Lagendre polynomials, Spherical harmonics, Angular momentum operator L2 and Lz, Space quantization. H atom, the R equation, Laguerre equation and Laguerre polynomials wave equation and energy of H like systems, Radial function and radial distribution functions, Shapes of s, p, d and f atomic orbitals.

Unit 3 Quantum Chemistry 3

Postulate of electron spin - orbital and spin functions. Many electron atoms. Approximation methods: Variation theorem and its proof, application to particle in one dimensional box, Helium atom. Perturbation method, First order perturbation, Application to helium atom, Hartree Fock Self Consistent Field method, Slater's treatment of complex atoms, Slater orbitals. Pauli principle, Slater determinant and wave function.

Unit 4 Quantum chemistry 4

Chemical boning, Born Oppenheimer approximation, Molecular orbital method for diatomic molecules, Correlation diagram, Non-c rossing rule. Valence bond method. Comparison of VB and MO method, Bonding in simple molecules like water, BF3, NH3 CH4, VSEPR theory, Pi bonding in simple molecules.

HMO method for linear conjugated hydrocarbons, aromatic hydrocarbons, calculation of free valence charge density and reactivity.

Unit 5 Electrochemistry 1

Activity and Activity coefficient of electrolytes, ionic strength, Debye Huckel theory of strong electrolytes . Debye Huckel limiting law, Mean ionic activity coefficient. Application of Debye Huckel theory to conductance bahaviour, Relaxation and electrophoretic effect, Debye-Huckel-Onsager equation and its derivation. Debye Falkenhagen effect . Wein effect.

Unit 6 Electrochemistry 2

Equilibrium Electrochemistry, EMF Phenomena, Cell Potential and its measurement, reference electrodes. Calculation of thermodynamic properties and activities. Cells without liquid junction potential. Liquid junction potential and its determination. Determination of solubility. pH Conductometric, Potentiometric and pH titrations, Redox indicators and redox titrations. Dynamic Electrochemistry, Electrical double layer, Various models of electrical double layer, Electrode polarization. Overpotertial and its theories, Butler Volmer equation, Tafel equation. Tafel plot and its significance

Corrosion and methods for prevention. Porbaux diagram and Evans diagrams. Storage cells, Lead acid battery, Lithium battery, nickel cadmium cell. Fuel Cell. Theory and working of fuel cell. H_2- O_2 fuel cell, methanol fuel cell, Solid oxide fuel cells.

References:

1 I. N. Levine , Quantum Chemistry, 6th Edn., Pearson Education, London, 2008
2 D. A. McQuarrie , Quantum Chemistry , 3rd Edn., Univ. Sci. Books, Mill Valley, California, 1983
3 J. P. Lowe, Quantum Chemistry 3rd Edn., Academic Press, New York, 2008
4 D. D. Fitts, Principles of Quantum Mechanics as Applied to Chemistry and Chemical Physics, CUP, Cambridge, New York, 2002
5 M. Taketani, The Formation and Logic of Quantum Mechanics, Vol. I-III, World Scientific, New Jersey,2001
6 G. Esposito, G. Marmo and G. Sudarshan, From Classical to Quantum Mechanics. An Introduction to the Formalism, Foundations and Applications, Cambridge, 2004
7 L. Piela, Ideas of Quantum Chemistry, Elsevier, Amsterdam, 2007
8 P. W. Atkins, Molecular Quantum Mechanics, OUP, Oxford, 1983
9 P.W. Atkins, Physical Chemistry, 8th Edn., Wiley, New York, 2006
10 J. Bockris and A.K.N. Reddy, Modern Electrochemistry, 2B, 2nd Edn., Wiley, New York, 1998
11 D .R. Crow, Principles and Applications of Electrochemistry, Chapman & Hall, 3rd Edn., New York, 1994

CORE

CHE 2104 Group Theory & Spectroscopy

(4 Credit) **64 hours**

Unit- 1

Molecular symmetry: Symmetry elements and operations, Point groups, Matrix representation of symmetry operations, character, Application of Group theory to symmetry properties of molecules, Definition of a mathematical group, Abelian group, cyclic group, symmetry operations as group elements, similarity transformation and classes Group multiplication table – Symmetry classification of molecules into point groups (Schoenflies symbol)- Application of symmetry to predict polar and chiral compounds.

Unit- 2

Reducible and Irreducible representations - Great Orthogonality theorem and its consequences (statement only, proof not needed), Character tables- reduction formula- Construction of character tables for point groups with order≤6- Interpretation of character tables. Wave functions as bases for irreducible representations, Construction of hybrid orbitals for AB_3(planar), AB_4(Td), AB_5(D3h) and AB_6(Oh) type of molecules - Symmetry adapted linear combinations, Projection operators, Application of projection operators to pi-bonding in ethylene, cyclopropenyl systems and benzene.

Unit 3

Nature of electromagnetic radiation, its interaction with matter, intensity and width of spectral lines, Classical and quantum chemical approach to absorption of radiation by molecules. Energy levels in molecules. Population of energy levels. Induced quantum transitions. Integrated absorption coefficient. Einstein's coefficients of absorption. Basis of selection rules, transition moment integral. Beer's Law. Induced absorption and emission of radiation by molecules.

Unit 4

Rotational and vibrational energies of diatomic molecules. Linear molecules. Symmetric top and asymmetric top molecules. Rotation spectra: Diatomic and polyatomic molecules. Vibration spectra of diatomic molecules, rotational character of vibration spectra. Coupling of rotation and vibration. Parallel and perpendicular bands. Morse potential of real molecules, overtones and combination, Fermi resonance.

Vibration spectra of polyatomic molecules, Normal modes of vibrations of polyatomic molecules. Raman Spectroscopy. Rotational Raman spectra. Vibrational Raman spectra, Surface enhanced Raman spectra, Resonance Raman, mutual exclusion principle. Applications of Group theory for molecular vibrations, The Characters for the Reducible Representation of Molecular Motion. The Symmetry of Group Vibrations. Selection rules and applications to IR and Raman spectra.

Fourier Transformation in IR spectroscopy, ATR. Temperature effects. Solid state spectroscopy. Diffuse reflectance spectroscopy.

Unit 5

Electronic energy states of molecules. Vibrational structure of electronic bands. Electronic transitions and absorption bands. Electronic spectra of diatomic and polyatomic molecules, its relation to electronic arrangement and symmetry of molecules. Different types of electronic transitions, Applications of group theory in electronic spectra, Electronic spectra of conjugated systems. Electronic spectra of coordination compounds.

Unit 6

Magnetic resonance spectroscopy : Theory of nuclear magnetic resonance, Chemical shifts, relaxation effects. Fourier Transformation in NMR, Measurement of relaxation time, Spin echo, NOE, 2D NMR. Electron spin resonance and applications. NQR Spectrosopy. MRI, Solid state NMR.

References:

1. F. A. Cotton, Chemical Applications of Group theory, Wiley Eastern, Singapore, 2nd Edn. 1992.
2. V. Ramakrishnan & M. S. Gopinadhan, Group theory in Chemistry, Vishal Pub. New Delhi, 1996
3. P. W. Atkins, Physical Chemistry 8th Edn. W. H. Freeman, New York, 2006
4. R. A. Alberty, Physical Chemistry 8th Edn., Wiley, New York., 1994
5. G. M. Barrow, Introduction to Molecular Spectroscopy, Mc Graw Hill, New York, 1962

6. C. N. Banwell: Fundamentals of Molecular Spectroscopy, 4th edn. Tata McGraw Hill, 1996
7. A. E. Derome: Modern NMR Techniques for Chemical Research, Pergamon Press, 1987
8. R. S. Drago: Physical Methods for Chemists, Second Edition, Saunders College Publication.1983
9. D. H. Williams and I. Flemming: Spectroscopic Methods in Organic Chemistry, Fourth Edition, McGraw-Hill, 1985
10. H. Gunther: NMR Spectroscopy, Second Edition, John Wiley. 2005
11. Norman B. Colthup , Lawrence H. Daly, Stephen E. Wiberley , Introduction to Infrared and Raman Spectroscopy, 3rd edition 1982

CORE

CHE 2105 Inorganic Chemistry Lab
(2 Credit)

Reactions of titanium , vanadium, chromium, manganese, iron, cobalt, nickel and copper ions Reactions of some less common metal ions (Tl, W, Mo, V, Zr, Th, U). The spot test technique for metal ions. Semimicro qualitative analysis of common and rare cations in a mixture. Ion exchange separations (Zn2+, Mg2+). Solvent extraction (Fe). An open-ended experiment involving analysis (e.g., Double salt formation and ion-exchange separation of oxidation states).

Estimation of metal ions by complexometric and cerimetric titrations. Estimation of Mg, Ca, Mn, hardness of water.

Synthesis of inorganic complexes and their characterization by various physicochemical methods, such as IR, UV, Visible, NMR, magnetic susceptibility etc. Selection can be made from the following or any other complexes for which references are available in the literature
Tris(oxalato)manganese(III)
Tetrapyridinesilver(II)peroxidisulphate
Tris(acetylacetonato) iron(III)
Bis(N,N-diethyldithiocarbamato)nitrosyliron(I)
Optical isomers of tris(ethylenediamine)cobalt(III)chloride
Nitropentamminecobalt(III) chloride
Nitritopentamminecobalt(III) chloride
Tri(acetylacetonato)manganese(III)
Tris(thiourea) copper(I) sulphate
Phenyl lithium
Tetraphenyl lead
Ferrocene
Phosphonitrilic chloride
Anhydrous copper(II) nitrate
Interpretation of its electronic spectrum and calculation of Dq values
Determination of crystal field splitting energy for certain ligands and construction of a part of the spectrochemical series
Methods for obtaining single crystals and checking the suitability of the crystals for single crystal determination.
Cobalt (II) bromide catalyzed oxidation of p-xylene

References:

1. G. Pass & H. Sutcliffe. Practical Inorganic Chemistry 2nd Ed., Chapman & Hill. 1974.
2. G. Marr & B. W. Rockett. Practical Inorganic Chemistry, Van Nostrand, 1972.

ELECTIVE

CHE 2106 Physical Chemistry-Equilibrium Thermodynamics

(2 Credit) **32 hours**

Unit 1

Mathematical techniques: Variables of thermodynamics, theoretical methods, Practical techniques. First and second laws of thermodynamics, thermodynamic functions, heat capacity, thermochemistry. Need for second law of thermodynamics. Entropy and free energy functions. Calculation of changes in thermodynamic function for ideal and non-ideal gases in isothermal and adiable process. Relation between thermo dynamic functions. Maxwell relations. Joule Thomson effect. Coefficient of thermal expansion and compressibility factor.

Unit 2

Applications of free energy function to physical and chemical charges. Equilibrium in chemical reactions. Third law of thermodynamics: Need for third law Calculation of absolute entropy, unattainability of absolute zero. Thermodynamic systems of variable composition Fugacity functions. Partial molar quantities; Thermodynamics of ideal solutions, real solutions and regular solutions. Dilute solutions of nonelectrolytes, Henry's law, Raults law. Gibbs Dehem equations. Duhem Margules equations. Activity and standard states of nonelectrolytes, Phase rule – Application to one, two and three component systems. Liquid-vapour equilibria of binary systems.

References:

1. Peter Atkins and Julio de Paula, Physical Chemistry, 7th edition or higher, Oxford.
2. I.M.Klotz & R.M.Robsenberg "Chemical Thermodynamics", 3rd Edn. W.A.Benjamin, INC.
3. L.K.Nash, "Elements of Chemical Thermodynamics" Addison Wesley.
4. Prigogine, Introduction to thermodynamic irreversible processes, Interscience.

ELECTIVE

CHE 2107 Stereochemistry and Conformational Analysis

(2 Credit) **32 Hours**

Unit 1

Geometrical isomerism, origin – structural features including C-C and C-hetero atom double bonds, cyclic systems and other systems exihibiting restricted rotation, different nomenclature including, cis-tarns, E,Z, syn-antae, endo-exo, relative acidity of maleic and fumeric acids.

Unit 2

Optical isomerism, origin of chirality, chiral centres, axes and planes, helicity, enantiotopic and diastereotopic atoms, groups and faces, prochiral centres and faces, allenes, cumulenes, biphenyls, and spirans. Compounds containing chiral atoms other than carbon.

Unit 3

Conformational analysis, Acyclic sp3–sp3, sp3-sp2 systems, structure and stability of small, medium, and large rings, cyclohexane, substituted cyclohexanes, A values, cyclohexene, decalins, bicyclic systems, anomeric effect,

Unit 4

Strain, types of strain including B, F, I, Pitzser strain, Beyer strain, conformation and reactivity.

References:

1. J. March: Advanced organic chemistry-reactions mechanisms and structure, 4th Ed., John Wiley
2. E. V. Anslyn and D. A. Dougherty: Modern Physical Organic Chemistry. University Science Books, 2006 edition.
3. T. H. Lowry and K. S. Richardson: Mechanism and Theory in Organic Chemistry, 3rd Ed., Addison-Wesley
4. F. A. Carey and R. J. Sundberg: Advanced Organic Chemistry, 5th Edition Plenum Press.
5. N. S. Issacs: Physical Organic Chemistry, Second Edition, John Wiley and Sons
6. A. Pross: Theoretical and Physical Principles of Organic Chemistry, John Wiley
7. P.S.Kalsi: Stereochemistry, Conformation and Mechanism, 3rd Edn., New Age Publications
8. E. L. Eliel and S. H. Wilen: Stereochemistry in Organic Compounds, John Wiley.
9. J. Clayden, N. Green, S. Warren and P. Wothers: Organic Chemistry, Oxford University Press
10. S. H. Pine: Organic Chemistry McGraw Hill
11. I. Flemming: Frontier Molecular Orbitals in Organic Chemistry, John Wiley
12. J. McMurry, Organic Chemistry (Fifth Edition), Brroks/Cole

ELECTIVE

CHE 2108 Nuclear Chemistry

(2 Credit) **32 Hours**

Unit 1

Radius of atomic nuclei: binding energy of nuclei, force between nucleons. Nuclear moment: nuclear angular momentum, nuclear magnetic dipole moment, electronic quadrupole moment – NQR Nuclear models: liquid drop model, nuclear shell model, fermi gas model. The subatomic particles: electron, proton, neutron, antiproton, positron, meson, quacks. Mass of nuclei: isotopes, isobars, mass spectrometry- identification of isotopes.

Unit 2

General characteristics of radioactive decay, parent-daughter decay growth relationships Decay kinetics, artificial transmutation and artificial radioactivity, nuclear stability and nuclear binding energy, packing fraction,

Unit 3

Types of nuclear reactions: react ion cross sect ion-compound nucleus theory, high energy nuclear, direct nuclear, photonuclear and thermonuclear react ions. Source of nuclear bombarding particles: Charged particle accelerators, gamma ray, X-ray and neutron sources. Fission: Fission products and Fission yield

curve, Fission energy, theory of nuclear fission, nuclear reactor, breeder reactor - nuclear reactors in India. Fusion reactions, hydrogen bomb and energy of sun.

Unit 4

Transuranium elements: Synthesis, separation and properties of transuranium elements.
Reprocessing of spent fuels. Solvent Extraction - Specific sequestering agents for transuranium elements.

Unit 5

Radio isotopes: Co-precipitation, ion-exchange, solvent extract ion - as a tracer, Synthesis of labeled compounds (any two), isotopic dilution and radiopharmaceuticals. Neutron activation analysis, positron annihilation and autoradiography. Dating of objects and mechanistic study. Radio isotopes: Co-precipitation, ion-exchange, solvent extraction - as a tracer, Synthesis of labeled compounds (any two), isotopic dilution and radiopharmaceuticals. Neutron activation analysis, positron annihilation and autoradiography.

Principles of determination of age of rocks and minerals, radio carbon dating principles, Isotope dilution and neutron activation analysis.

References:

1. H. J. Arnikar, "Essentials of Nuclear Chemistry", Wiley Eastern Ltd., New Delhi (1982)
2. A.K. Srivatsava and P. Jain, "Essential of nuclear Chemistry", S.Chand, N.Delhi, 1989
3. G.R. Choppin, "Radiochemistry and Nuclear chemistry", 2002.
4. G. Friedlander, J. W. Kennedy, and J. M. Miller, "Nuclear and Radiochemistry", John Wiley and Sons Inc., Japan Second Edition (1964)
5. S. Glasstone, "Source book on Atomic Energy", Van Nostrand Co. Inc., New Jersey, Second Edition (1958)
6. R. Gopalan, "Elements of nuclear chemistry", Sultan Chand, Delhi, 2000.

ELECTIVE

CHE 2109 ENVIRONMENTAL CHEMISTRY

(2 Credit) **32 Hours**

Unit 1

Global warming – Ozone hole. Environmental segments – The hydrological cycle – The oxygen cycle – The nitrogen cycle – The sulphur cycle – Composition of atmosphere – Earth's radiation balance – Green house effect.

Unit 2

Air pollution – Primary pollutants, Acid rain – Air quality standards – Sampling – Monitoring – Analysis of CO, nitrogen oxides, sulphur oxides, hydrocarbons and particulate matter – Control of air pollution.

Soil pollution – Inorganic and organic components in soil – Acid – Base and ion exchange reactions in soils – Micro and macro nutrients – Wastes and pollutants in soil.

Unit 4

Water pollution – Water pollutants – Eutrophication – Water quality criteria for domestic and industrial uses – Trace elements in water – Determination of quality parameters – Total hardness, TDS, pH, chloride, heavy metals, etc.

Principles of water and waste water treatment – Aerobic and anaerobic treatment – Industrial waste water treatment – Removal of organic and inorganic materials from water and waste water.

Unit 5

Instrumental techniques in environmental analysis – Use of neutron activation analysis – ASV, AAS, GC, HPLC, ion selective electrodes and ion chromatography in environmental chemical analysis.

References:

1. Environmental Chemistry , Gary W. VanLoon, Stephen J. Duffy, Oxford University Press, 2005
2. Principles Of Environmental Chemistry, James Girard, Jones & Bartlett Learning, 2005
3. Environmental Chemistry, Seventh Edition, Stanley E. Manahan, CRC Press, 2010
4. Applications of Environmental Chemistry, Eugene R. Weiner, CRC Press,2010
5. Environmental chemistry, Ian Williams, J. Wiley, 2001
6. The essential guide to environmental chemistry, Georg Schwedt, John Wiley, 2001

ELECTIVE

CHE 2110 CHEMISTRY OF POLYMERS

(2 Credit) **32 Hours**

Unit 1

History of Polymer Science. Concept of macromolecules, Principle of duality, Integration of molecular character and material character. Molecular design, synthesis and process technologies. Nomenclature and Classification. Raw Material sources of polymers. Natural gas, coal and petroleum. Monomers and polymers derived from natural gas. Petroleum and petrochemicals. Monomers and polymers derived from ethylene and propylene. Monomers and polymers derived from C4 and C5 Systems and BTX fraction. Acetylene as a source of monomers.

Unit 2

Polymerization processes. Free radical addition polymerization. Kinetics and mechanism. Chain transfer. Molecular weight distribution and molecular weight control. Cationic and anionic polymerization. Polymerization without termination. Living polymers. Step Growth polymerization. Kinetics and mechanism. Linear Vs cyclic polymerization, Group Transfer, metathesis and ring opening polymerization. Copolymerization. The copolymerization equation, Q-e scheme, Gelation and Crosslinking. Copolymer composition drift. Polymerization techniques. Bulk Solution, melt, suspension, emulsion and dispersion techniques

Unit 3

Polymer Stereochemistry. Organizational features of polymer chains. Configuration and conformation, Tacticity, Repeating units with more than one asymmetric center. Chiral polymers – main chain and side chain. Stereoregular polymers. Manipulation of polymerization processes. Zeigler-Natta and Kaminsky routes. Coordination polymerization. Metallocene and Metal oxide catalysts.

Unit 4

Polymer Characterization. Molecular weights. Concept of average molecular weights, Determination of molecular weights. GPC and Light scattering techniques. Molecular weight distribution. Crystalline and amorphous states. Glassy and Rubbery States. Glass transition and crystalline melting. Spherullites and Lammellae. Degree of Crystallinity, Thermal analysis of polymers. TG/DTG, DTA/DSC, Spectroscopy of polymers. Microstructure determination by IR, Raman, UV, NMR and MS techniques. Solid State NMR and polymer stereochemistry.

Unit 5

Industrial polymers. Synthesis, Structure and applications. Polyethylene, polypropylene, polystyrene. PVC, PVA, PAN, PA. Poly(vinyl carbazole), poly(vinyl imidazole). PMMA and related polymers. Flourine containing polymers. Reaction polymers. Polyamides, polyesters. Epoxides, polyurethanes, polycarbonates, phenolics, PEEK, Silicone polymers. Reactions of polymers. Polymers as aids in Organic Synthesis. Polymeric Reagents, Catalysts, Substrates, Liquid Crystalline polymers. Main chain and side chain liquid crystalline polymers.

References:

1. F.W. Billmayer. Textbook of Polymer Science. 3rd Edn, Wiley. N.Y. 1991.
2. J.M.G Cowie. Polymers: Physics and Chemistry of Modern Materials. Blackie. London, 1992.
3. R.J.Young, Principles of Polymer Science, 3rd Edn. , Chapman and Hall. N.Y. 1991.
4. P.J. Flory. A Text Book of Polymer Science. Cornell University Press. Ithacka, 1953.
5. F. Ullrich, Industrial Polymers, Kluwer, N.Y. 1993.
6. H.G.Elias, Macromolecules, Vol. I & II, Academic, N.Y. 1991.
7. J.A.Brydson, Polymer chemistry of Plastics and Rubbers, ILIFFE Books Ltd., London, 1966.

CORE

CHE 2201 ANALYTICAL CHEMISTRY

(2 Credit) **32 Hours**

Unit 1

Evaluation of analytical data, significant figures. Precession- Standard deviation, coefficient of variation – statistical treatment of data-students T test, rejection of suspected value, Q test.

Classical methods of Analysis, Titrimetry – Theory of indicators- Gravimetry- Theory of complexometric titrations-metal-ion indicators Masking and demasking-Applications of Complexometric Titrations.

Unit 2

Separation Techniques. Distribution law-Liquid-liquid extractions, synergistic extraction. Countercurrent extraction, super critical fluids, Electrophoresis- theory and applications.

Chromatography-classification-column-paper and thin layer chromatography. HPLC-Outline study of instrument modules. Ion – exchange chromatography-Theory. Important applications of chromatographic techniques. Gel Permeation Chromatography.

Unit 3

Gas chromatography – basic instrumental set up-carriers, columns, detectors and comparative study of TCD, FID, ECD and NPD. Qualitative and quantitative studies using GC, Preparation of GC columns, selection of stationary phases of GLC, CHN analysis by GC. Super Critical Fluid Chromatography.

Unit 4

Radiochemical Methods in Analysis – isotopic dilution analysis-Activation analysis, Radiometric titrations-Applications.

Thermal methods of Analysis TG, DTA and DSC - Instrumentation and Theory – Factors affecting TGA - effect of atmosphere on DTA. TG of copper sulphate pentahydrate and calcium oxalate monohydrate. Application of thermal methods for identification of substances.

Unit 5

Spectrophotometric Analysis - UV-VIS and IR Spectrophotometry. Basic instrumentation for UV-Vis and IR spectrophotometry-single beam and double beam instruments, FT-IR, Fundamental laws of photometry-deviations from Beers law - photometric accuracy-relative photometric error. – Simultaneous determination of two components-.

References:

1. D.A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, Fundamentals of Analytical Chemistry, 8th Edn., Saunders College Pub., 2007.
2. Analytical Chemistry, Gary D Christian, John Wiley & Sons, 2007, 6th edition
3. Principles of Analytical Chemistry, Miguel Valcarcel Cases, Springer, 2000
4. Analytical Chemistry, Jean- Michel Mermet, Matthias Otto, Robert Kellne Wiley-VCH, 2004
5. Handbook of Analytical Techniques, Volume 2, Helmut Gunzler, Alex Williams. Wiley-VCH,2001
6. Analytical chemistry, Seamus Higson, OUP Oxford, 2003
7. Reference Materials in Analytical Chemistry, Adolf Zschunke, Springer, 2000

CORE

CHE 2202 Inorganic Chemistry-II

(3 Credit) **48 Hours**

Unit 1

Splitting of d orbitals in different crystal fields such as octahedral, tetragonal, square planar, tetrahedral trigonal bipramidal and square pyramidal fields. Energy levels of d orbitals in crystal fields of different symmetries crystal field stabilization energy and its calculations. Thermodynamic effects of LFSE. Factors affecting the splitting parameter. Spectrochemical series. Molecular orbital theory based on group theoretical approach and bonding in metal complexes. σ and π bondings in complexes. MO diagrams of complexes with the without π bonds. Effect of π bond on the stability of σ bond. Nephelauxetic series.

Unit 2

Electronic Spectra of complexes: Term symbols of d^n system, Raccah parameters, splitting of terms in weak and strong octahedral fields. Correlation diagrams for d^n and d^{10-n} ions in octahedral and tetrahedral fields (qualitative approach), d-d transition, selection rules- effect of spin-orbit coupling Orgel diagrams- splittings for d^1, d^9 and high spin d^4 and d^6, splittings for d^2, d^3,d^8 and high spin d^7 (ii) Tanabe-Sugano diagrams-spectra of d7, d5 and low spin d6 complexes., Calculation of Dq, B and β (Neplauxetic ratio) values. Spectra of complexes with lower symmetries. Jahn Teller effect and their consequences on the nature of the electronic spectra Charge transfer spectra electronic spectra of lanthanide and actinide complexes

Unit 3

Types of magnetic behaviour, magnetic susceptibilities, Pascal's constants, paramagnetism in experimental simple systems where S = ½, van Vleck's equation, its derivation and its applications. Spin-orbit coupling

and susceptibility of transition metal ions and rare earths; magnetic moments of metal complexes with crystal field terms of A, E and T symmetry, T.I.P., intramolecular effects, antiferromagnetism and ferromagnetism of metal complexes, super paramagnetism. High and low spin equilibria. Magnetic properties of lanthanides and actinides

Unit 4

Electronic paramagnetic resonance spectroscopy: Electronic Zeeman effect, Zeeman Hamiltonian and EPR transition energy. EPR spectrometers, presentation of spectra. The effects of electron Zeeman, nuclear Zeeman and electron nuclear hyperfine terms in the Hamiltonian on the energy of the hydrogen atom. Shift operators and the second order effect. Hyperfine splittings in isotropic systems, spin polarization mechanism and McConnell's relations Anisotropy in g-value, EPR of triplet states, zero field splitting, Kramer's rule, survey of EPR spectra of first row transition metal ion complexes.

Unit 5

Thermodynamic and kinetic stability. Kinetics and mechanism of nucleophilic substitution reactions in square planar complexes. Mechanism of entering and other leaving groups and trans effect. Kinetics and mechanism of octahedral substitution.-Dissociative and associative mechanisms, base hydrolysis, Racemization reactions, Trans effect, trans effect series, and theories of trans effect Electron transfer reactions-outer sphere mechanism-Marcus theory, inner sphere mechanism.

References:

1. F. A. Cotton, G. Wilkinson, C. A, Murillo, and M. Bochmann Advanced Inorganic Chemistry, 6th Edition Wiley-Interscience: New York, 1999.
2. J.E. Huheey, Ellen A. Keiter and Richard L. Keiter "Inorganic Chemistry, Principles of structure and Reactivity", 4th Ed., Harper Collin College Publishers, 1993
3. J. W. Steed, J. L. Atwood, Supramolecular Chemistry, 2nd edition, John Wiley & Sons Ltd., (2009)
4. D. F. Shriver, P. W. Atkins, C. H. Langford, Inorganic Chemistry, 3rd Ed. ELBS, 1999.
5. B. Douglas, D. McDaniel, J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Ed., Wiley.
6. N. N. Greenwood, A. Earnshaw, Chemistry of the Elements, 2nd Edn., BH, 1997.

CORE

CHE 2203 Organic Chemistry II

(4 Credit) **64 Hours**

Unit 1 (15 Hours)

Reagents for oxidation and reduction: PCC, activated DMSO oxidations, osmium tetroxide, selenium dioxide, singlet oxygen, peracids, hydrogen peroxide, periodic acid, lead tetraacetate., Woodward and Prevost hydroxylation, Sharpless asymmetric epoxidation. Catalytic hydrogenations (heterogeneous and homogeneous), metal hydride reduction, Birch reduction, hydrazine and diimide reduction.

Synthetic applications of organometallic and organo-nonmetallic reagents: Reagents based on chromium, nickel, palladium, silicon, and born, Gilman's reagent, phase transfer catalysts, hydroboration reactions, synthetic applications of alkylboranes.

Unit 2 (12 Hours)

Chemistry of carbonyl compounds: Reactivity of carbonyl groups in aldehydes, ketones, carboxylic acids, esters, acyl halides, amides. Substitution at α-carbon, aldol and related reactions, Claisen, Darzen, Dieckmann, Perkin, Prins, Mannich, Stork-enamine reactions. Conjugate additions, Michael additions and Robinson annulation. Reaction with phosphorous and sulfur ylides.

Unit 3 (14 Hours)

Protecting groups, functional group equivalents, reversal of reactivity (Umpolung)
Synthetic strategies: Introduction to retrosynthesis, strategic bond analysis, synthesis of longifolene, Corey lactone, Djerassi Prelog lactone
All students to give a presentation ($^1/_2$ hr.) of a multistep synthesis.

Unit 4 (9 Hours)

Rearrangements involving electron deficient carbon and nitrogen. Mechanism of the following rearrangements: Wagner-Meerwein, Pinacol, Demyanov, dienone-phenol, Favorskii, Wolff, Hofmann, Curtius, Lossen, Schmidt, Beckmann, benzidine, and Hofmann-Loffler rearrangements. Fritsch-Buttenberg-Wiechell rearrangement, Corey-Fuchs reaction, Seyferth-Gilbert homologation, Grubbs catalysts and olefin metathesis.

Unit 5 (14 Hours)

Pericyclic reactions, study of the principle of conservation of orbital symmetry, selection rules (ground and excited states), electrocyclic reactions, cycloadditions, cheletropic reactions, sigmatropic rearrangements – Cope rearrangement, Claisen rearrangement, and ene-reaction, secondary orbital interactions in [4+2] cycloadditions, Intramolecular Diels–Alder reactions.
Photochemistry: Unimolecular and bimolecular processes in the excited states, mechanism of important photochemical reactions, Paterno-Buchi reaction, Norrish Type I and Type II fragmentation, di-pi-methane rearrangement, Barton reaction, photochemistry of arenes, cyclohexadienones and furanones, nitrocompounds

References:

1. M. Smith: Organic Synthesis, McGraw-Hill.
2. T.W.Greene and PG M Wuts:Protecting Groups in Organic Synthesis,2nd ed., John Wiley
3. J. March: Advanced Organic Chemistry-Reactions, Mechanisms and Structure, 4th ed., John Wiley
4. T H.Lowry and K.S.Richardson:Mechanism and Theory in Organic Chemistry, 3rd ed.
5. F. A. Carey and R. J. Sundberg: Advanced Organic Chemistry (parts A and B), Third Edition Plenum Press.
6. A. Pross: Theoretical and Physical Principles of Organic Chemistry, John Wiley
7. T.W. Graham Solomons:Fundamentals of Organic Chemistry, 5th ed., John Wiley
8. S. Warren: Organic Synthesis: The Disconnection Approach, John Wiley
9. H. O. House: Modern Synthetic Reactions, W. A. Benjamin
10. W.Carruthers:Some Modern Methods of Organic Synthesis,Cambridge University Press.
11. I. L. Finar: Organic Chemistry Volumes 1 (6th ed.), Longman.
12. I. Flemming: Frontier Orbitals and Organic Chemical Reactions, John Wiley
13. J. Clayden, N. Green, S. Warren and P. Wothers: Organic Chemistry, Oxford University Press
14. N. J. Turro: Modern Molecular Photochemistry, Bejnjamin/Cummings

CORE

CHE 2204 Physical chemistry II

(3 Credit) **48 Hours**

Unit 1 Statistical Thermodynamics 1

Thermodynamic probability, microstate and macrostate, entropy and probability, most probable distribution, residual entropy and its calculation. Maxwell - Boltzman statistics. Derivation of Maxwell's distribution of molecular velocities from Maxwell -Boltzman distribution law. Effect of temperature on distribution. Calculation of most probable velocity, average and mean square velocity, components of velocity. Mean free path, Effusion and diffusion, thermal conductivity and viscosity of gases.

Unit 2 Statistical Thermodynamics 2

Partition function and its relation to thermodynamic properties, Translational , rotational and Vibrational partition function. Molecular partition function for delocalized systems, calculation of equilibrium constant using partition functions. Heat capacity of gases, Anomalous heat capacity of H_2 Heat capacity of solids: Dulong - Petits law, Einstein's theory and its modification, Debye's theory of heat capacity of solids.

Unit 3 Statistical Thermodynamics 3

Quantum statistics, Bose - Einstein statistics, Fermi - Dirac statistics, Comparison of Maxell - Boltzman, Bose=- Einstein and Fermi - Dirac Statistics, Dilute Systems. Application of Bose -Einstein Statistics, Gas degeneration, Application to liquid helium, Bose Einstein Condensation. Application of Fermi -Dirac Statistics to electrons in metals, Extreme Gas Degeneration, Electron gas in metals and its contribution to pressure and heat capacity.

Unit 4 Statistical Thermodynamics 4

Partition function for systems of dependent particles, Configurational integral and configurational partition function. Imperfect gas, Van der waals equation and Virial equation of state, Evaluation of the first virial coefficient. Condensed state, Cluster integrals, Communal entropy.

Unit 5 Linear Non-equilibrium thermodynamics

General theory, Local entropy production, balance equation for concentration. Energy conservation in open systems. Entropy balance equation. Forces and Fluxes, Steady state and local equilibrium conditions. Linear phenomenological laws. Phenomenological coefficient, Systems with heat, matter and electrical transport, Onsager Reciprocal relation, Application to Diffusion -Thermal diffusion, Thermal Osmosis and electrokinetic effects, Soret Coefficient, Seebeck effect.

Unit 6 Order through Fluctuations

Nonlinear thermodynamics- Far from equilibrium systems- entropy production- stability of non-equilibrium stationary states- linear stability analysis. Dissipative structures- constructive role of irreversible processes- loss of stability, bifurcation and symmetry breaking. Breaking of Chiral symmetry and life- chemical oscillations. Turing structures and propagating waves. Structural instability and biochemical evolution.

References:

1. F.W. Sears, Introductions to Thermodynamics, Kinetic Theory of Gases and Statistical Mechanics, Addision Wesley Pub. Cambridge, 1998.
2. F.C. Andrews, Equilibrium to Statistical Mechanics, John Wiley, New York, 2002.
3. Malcolm Dole, Introduction to Statistical Thermodynamics, Prentice Hall, London, 1997.
4. L.K. Nash, Statistical Thermodynamics, Addison Wesley, New York, 1999.
5. J. Kestin and J.R. Dorfman, A course in Statistical Thermodynamics, Academic press
6. D. Kondepudi and I. Prigogine, Modern Thermodynamics: From Heat Engines to Dissipative Structures, Wiley, New York, 1998.
7. D. A. McQuarrie, Statistical Mechanics, Harper and Row, New York, 1976
8. I. Muller, A History of Thermodynamics. The Doctrine of Energy and Entropy, Springer, Berlin, 2007

CORE

CHE 2205 Organic Spectroscopy

(2 Credit) **32 Hours**

Unit 1: Ultraviolet-Visible Absorption and Emission and Chirooptical Spectroscopy

Energy levels and selection rules, Woodward-Fieser and Fieser-Kuhn rules, estimation of λmax of substituted aromatic ketones, aldehydes and acids.

Influence of substituent, ring size and strain on spectral characteristics. Solvent effect, Non-conjugated interactions. Spectral correlation with structure. ; Brief Introduction to emission spectroscopy ORD, CD, Octant rule, axial haloketone rule, Cotton effect.

Unit 2: Infrared Spectroscopy

Fundamental vibrations, overtones, Fermi Resonance, Advantages of FT technique, Characteristic regions of the spectrum. Influence of substituents, ring size, hydrogen bonding, vibrational coupling, hybridization and field effect on frequency. Determination of Stereochemistry.
IR spectra of chemical classes including minoacids.

Unit 3: Nuclear Magnetic Resonance Spectroscopy

Magnetic nuclei with special reference to 1H and 13C nuclei. Chemical shift and shielding/deshielding, relaxation processes, chemical and magnetic non-equivalence, local diamagnetic shielding and magnetic anisotropy. Proton and 13C NMR scales, characteristics of 13C as a nucleus.
Spin-spin splitting, AX, AX2, AX3, A2X3, AB, ABC, AMX type coupling, First order and non-first order spectra, Pascal's triangle, coupling constant, mechanism of coupling, Karplus curve, quadrupole broadening and decoupling, diastereomeric protons, virtual coupling, long range coupling effects, NOE, coupling with other nuclei.

Simplification non-first order spectra to first order spectra, shift reagents-mechanism of action, spin decoupling and double resonance, Chemical shifts and homonuclear/heteronuclear couplings, the basis of heteronuclear decoupling.

2D NMR and COSY, HMBC, HMQC

Polarization transfer. Selective Population Inversion (qualitative description only), DEPT, sensitivity enhancement and spectral editing.

Unit 4: Mass Spectrometry

Molecular ion, ion production methods (EI). Soft ionization methods: FAB, CA, MALDI, PD, Field desorption electrospray ionization, HRMS and formula mass, Fragmentation patterns, nitrogen and ring rules, Rule of thirteen, McLafferty rearrangement, Applications. HRMS, MS- MS, LC-MS, GC-MS.

Unit 5: Structural Elucidation Using Spectroscopic Techniques

Identification of structures of unknown organic compounds based on the data from UV-Vis, IR, 1HNMR and 13CNMR spectroscopy.

References:

1. Introduction to Spectroscopy: A Guide for Students of Organic Chemistry (3rd Ed.), D.L.Pavia, G.M.Lampman, G.S.Kriz, Thomson. 2004.

2. Solving Problems with NMR Specroscopy, Atta-Ur-Rahman, M.I.Choudhary, Academic Press, New York, 1996.
3. Organic Structures from Spectra (fourth edition), L D Field;S Sternhell and J R Kalman;Wiley (2008)
4. Physical Methods for Chemist, R. S. Drago, Saunders, 1992.
5. Fundamentals of Molecular Spectroscopy, C. N. Banwell and E. M. McCash, 4th ed, McGraw-Hill, 1994.
6. Organic Spectroscopic Structure Determination: A Problem Based Learning Approach, D.F.Taber, Oxford University Press, 2009.
7. NMR Spectroscopy, H. Gunther, 2nd ed.; John Wiley and Sons, 1995.
8. Spectroscopic identification of organic compounds, R. M. Silverstein, G.C. Bassler, T. C. Morril, John Wiley, 1991.
9. Spectroscopic methods in organic chemistry, D. H. Williams, I. Fleming, Tata McGraw Hill. 1988.
10. Organic Spectroscopy, W. Kemp, 2nd edition, ELBS-Macmillan, 1987.
11. F. Bernath, Spectra of Atoms and Molecules, 2nd Edition, Oxford University Press, 2005.
12. E. B. Wilson, Jr., J. C. Decius and P. C. Cross, Molecular Vibrations: The Theory of Infrared and Raman Spectra, Dover Publications, 1980.
13. A. Weil and J. R. Bolton, (Eds), Electron Paramagnetic Resonance: Elementary Theory and Practical Applications, Second Edition, Wiley Interscience, John Wiley & Sons, Inc., 2007.
14. C. P. Slichter, Principles of Magnetic Resonance, Third Edition, Springer-Verlag, 1990.
15. H. Gunther, NMR Sprectroscopy: basic principles, concepts, and applications in chemistry Second Edition, Wiely 1997.
16. Spectral data bases (RIO DB of AIST, for example)

CORE

CHE 2206 Organic Chemistry Lab

(2 Credit)

Part 1 : General methods of separation and purification of Organic Compounds such as:
Solvent extraction
TLC and paper chromatography
Column Chromatography
Part 2: Separation and Identification of the components of organic binary mixtures.
Part 3 : Preparation of Organic compounds by Multistep reactions.*
Part 4 : Spectral interpretation of organic compounds, using UV-Vis and FTIR
Part 5 : Drawing the structures of organic molecules and reaction schemes by Chemdraw.
*Progress of the reactions should be followed by spectroscopic and chromatographic methods (UV-Vis, TLC, GC, HPLC, etc.,)
Computational Organic Chemistry Practicals
Construction of z-matrices
Structure drawing
Molecular Mechanics Calculations
Mapping molecular electrostatic potential
Calculation of Hückel Molecular Orbitals
Applications of Semi-Empirical and Ab Initio methods in calculating molecular orbitals and geometry optimization.

References:

1. R. Tastchell et al: Vogel's Textbook of Practical Organic Chemistry, 5th ed., John Wiley.

2. D. L. Pavia, G. M. Lampman and G. S. Kriz: Introduction to Organic laboratory Techniques, 3rd ed., Saunders Golden Sunburst Series
3. L. W. Harwood and C. J. Moody: Experimental Organic Chemistry-Principals and Practice, Blackwell Science Publications

ELECTIVE

CHE 2207 Introduction to Materials Chemistry

(2 Credit) **32 hours**

Unit 1

Chemistry of Materials. Historical perspectives – strategies for the design of new materials- a critical thinking approach. Ionic and covalent solids. Molecular and metallic solids. Amorphous and crystalline materials. Crystalline state. Structural organization of crystalline solids-theories of bonding. Crystal structures. Imperfections in crystal structures. Amorphous materials – glasses and ceramic solids. Structural organization of amorphous solids. Traditional ceramics. Synthetic high performance ceramics. Crystal structure of ceramics.

Unit 2

Metals and alloys. Structural and bonding theories of metals. Alloys -ferrous alloys – phase behavior of ferrous alloys. Behaviour of binary alloys. Intermediate compounds and intermediate phases. Nonferrous metals and alloys. Shape memory alloys. PZT materials. Optical, electrical and magnetic properties of metallic materials.

Unit 3

Semiconductor materials- properties and types of semiconductors. Structure and Bonding of semiconductor materials. Silicon based semiconductors. II-VI (wide band gap) and III-V (narrow band gap) compound semiconductors. Electrical, optical and magnetic properties of semiconductor materials. Preparation and properties of ZnO, ZnS, CdS, CdTe, Ga-As, In-S, Cu-In-S. Application in photovoltaic devices

Unit 4

Polymer Materials- classification and nomenclature of polymers. Methods of Polymerization. Dendritic and cascade polymers. Polymers via Click Chemistry. Properties of polymers. Plastics and elstomers. Viscoelastic behavior. Rubber like elasticity. Crystalline and amorphous polymers. Glass transition temperature and crystalline melting. Polymer composites- polymer matrix composites.

Unit 5

Nanomaterials. Materials in the nanodomain. Zero, one and two dimensional materials. Particle size dependent change in properties of materials. Metals in the nanodomain. Gold and silver nanoparticles. Preparation, properties and applications. Core shell structures. Semiconductor nanoparticles. Quantum dots. ZnO, ZnS, CdS and CdSe quantum dots. Electrical and optical properties. Nano domains of Carbon-fullerenes, carbon nanostructures, graphene.

Unit 6

Characterization of Materials. Optical Microscopy- Principles, instrumentation and application of confocal raman microscopy, SPM/STM. Electron microscopy- SEM, FESEM, TEM. Principles, instrumentation and applications. Surface and core level techniques- Photoelectron spectroscopy- X-Ray and UV. Thermal methods- TG/DTG, DTA, DSC, DMA. X-Ray Diffraction

References:

1. B. D. Fahlman, Materials Chemistry, 2nd Edn. Springer, Heidelberg, 2011
2. R. Zallen, Physics of Amorphous Solids, Wiley, New York, 1983
3. R. J. Borg, G. J. Dienes, The Physical Chemistry of Solids, Academic Press, Boston, 1993
4. D. Kingery, H. K. Bowen, D. R. Uhlmann, Introduction to Ceramics, 2nd Edn. Wiley, New York, 1992
5. 5. J. M. J. Cowie, Polymers. Physics and Chemistry of Modern Materials, 3rd Edn. CRC Press, Boca Raton, 2007
6. S. O. Kasap, Principles of Electronic Materials and Devises, Mc Graw Hill,2006

ELECTIVE

CHE 2208 Stereochemistry in Organic Synthesis

(2 Credit, Elective) **32 hours**

Unit 1

Reaction Mechanisms and Conformational Effects on Reactivity; Ester Hydrolysis, Alcohol Oxidations, SN2 Reactions, Elimination Reactions, Epoxidation by Intramolecular Closure of Halohydrins, Epoxide Openings (SN2), Electrophilic Additions to Olefins, Rearrangement Reactions, Pericyclic Reactions, Conformational and Stereoelectronic Effects on Reactivity,

Unit 2

Stereospecific and stereoselective synthesis, introduction to assymmentric synthesis, principles, general strategies, chiral pool-glucose, chiral auxiliaries-Diels alder reaction, , chiral reagents – Binol derivatives of LiAlH4, chiral catalysts – CBS catalyst, stereoselective reactions of enolates, enzyme-catalyst nexus, baker's yeast

References:

1. J. March: Advanced organic chemistry-reactions mechanisms and structure, 4th Ed., John Wiley
2. E. V. Anslyn and D. A. Dougherty: Modern Physical Organic Chemistry. University Science Books, 2006 edition.
3. T. H. Lowry and K. S. Richardson: Mechanism and Theory in Organic Chemistry, 3rd Ed., Addison-Wesley
4. F. A. Carey and R. J. Sundberg: Advanced Organic Chemistry, 5th Edition Plenum Press.
5. N. S. Issacs: Physical Organic Chemistry, Second Edition, John Wiley and Sons
6. A. Pross: Theoretical and Physical Principles of Organic Chemistry, John Wiley
7. P.S.Kalsi: Stereochemistry, Conformation and Mechanism, 3rd Edn., New Age Publications
8. E. L. Eliel and S. H. Wilen: Stereochemistry in Organic Compounds, John Wiley.
9. J. Clayden, N. Green, S. Warren and P. Wothers: Organic Chemistry, Oxford University Press
10. S. H. Pine: Organic Chemistry McGraw Hill
11. I. Flemming: Frontier Molecular Orbitals in Organic Chemistry, John Wiley
12. J. McMurry, Organic Chemistry (Fifth Edition), Brroks/Cole

ELECTIVE

CHE 2209 Crystallography

(2 credit) **32 Hours**

Unit 1

Concepts of Symmetry, point groups and space groups; crystal lattices; Elements of scattering theory, diffraction principles, reciprocal lattice

Unit 2

Methods of characterizing crystal structure, powder X-ray diffraction method

Unit 3

Single crystal X-ray diffraction. Data collection and processing strategies

Unit 4

Structure solution. Patterson and direct methods. Refinement techniques

Unit 5

Crystal growth techniques.

References:

1. R.S. Drago, "Physical Methods for Chemists", Sauders College Publishing
2. Crystal Structure Analysis – A Primer, J.P. Glusker and K.N. Trublood
3. C Giacavazzo (Ed.) Fundamentals of crystallography
4. J. D. Dunitz, X-ray analysis and the structure of organic molecules
5. G.H. Stout and L.H. Jensen, X-ray structure determination: A practical guide

ELECTIVE

CHE 2210 BIOANALYTICAL CHEMISTRY

(2 Credit) **32 Hours**

Unit 1-Biomolecules

Biomolecules- amino acid, protein, nucleic acid –structures, physical and chemical properties, features and characteristics of major biomolecules, structure-function relationship, significance.
Analyses and quantification of biomolecules- method to detect and quantify biomolecules.

Unit 2-Centrifugation and separation

Principle of centrifugation, concept of RCF, features and component of major types of centrifuge, preparative, differential and density gradient centrifugation, analytical ultra-centrifugation, centrifugation methods for bio analysis. Determination of molecular weight.

Unit 3-Electrophoresis

Electrophoretic techniques- Principles of electrophoretic separation. Types of electrophoresis including paper, cellulose, acetate/nitrate and gel. Electroporation, Pulse field gel electrophoresis- applications in life and health science.

Unit 4-Immunochemical techniques

Radio immune assay (RIA) - principle and applications. Enzyme linked immune sorbent assay (ELISA) principle and applications. Biosensors-applications

Unit 5-Electron microscopy

Transmission and scanning, freeze fracture techniques, specific staining of biological materials.

References:

1) Understanding bio analytical chemistry-principle and applications-Victor A. Gault and Neville. H. Mcclenaghan.John Wiley and Sons, Ltd Publications 2009
2) Bio analytical Chemistry- Andreas Manz.: Nicole Pamme. Dimitri Iossifidis.2004
3) Bio analytical chemistry- Suson R. Mikkelsen, Eduaro Corton- John Wiley and Sons, Ltd Publications
4) Practical Biochemistry-Principles and techniques: -Keith Wilson and John Walker 5th edition, cambridge University press (2000)

ELECTIVE

CHE 2211 Polymer composites

(2 Credit) **32 Hours**

Unit 1

Different types of polymerizations like addition, condensation and stereoregular polymerization. Initiators used, important steps involved, kinetics and mechanism of addition, condensation and stereoregular polymerizations. Copolymerization and its kinetics. Important techniques of polymerization such as emulsion, bulk, solution and suspension.

Unit 2

Polymer characterization, molecular weight determination by GPC,viscosity,light scattering and osmometry.Physical methods of polymer analysis such as IR,NMR,X-ray etc.Thermal analysis of polymers using DSC,TGA,DTA,DMA etc.

Unit 3

Polymer degradation and stabilization: Thermal, oxidative, photochemical and ozone degradation under special environments. Mechanism of different types of degradation. Commonly used anti-degradants and the mechanism of their stabilization.

Unit 4

Polymer materials- Production, Properties and Applications of-polyethylene, polypropylene, polystyrene, polyurethanes, polyacrylonitrile, polybutadiene, SBR,CR,NBR,EPDM,IIR

Unit 5

Introduction to composite materials- Classification, introduction to polymer composites-nano, micro and macro scales. Reinforcements-short fibre,long fiber and particulate fillers.Matrices-thermoplastics,thermosets and rubbers.Nano and microcomposites.Short and long fiber composites, treatment of reinforcements, polymer-filler interactions, use of coupling and bonding agents.

Unit 6

Additives used in rubber compounding: Curing systems, antidegradants, plasticizers, fillers, colourants, blowing agents etc.

References:

1. Polymer chemistry,Paul C. Hiemenz
2. Principle of polymer chemistry, P.J Flory
3. Experimental methods in polymer chemistry,J.F Rabek
4. Encyclopedia of polymer science and Engg.,Vol.15
5. Handbook of polymer synthesis ,Part A & B, Hans.R.Kricheldorf(ed)
6. A text book of polymer science, F.W Billmeyer
7. G.Lubin-Handbook of composites-Van Nostrand(1982)
8. R.Krishnamoorti & R.A Vaia Polymer nano composites: Synthesis characterization and modeling , American Chemical Society (2002)
9. Handbook of plastic test methods,R P Brown.The plastic and rubber institute,1981
10. Rubber technology and manufacture Blow C M

CORE

CHE 2301 INSTRUMENTAL METHODS OF ANALYSIS

(2 Credit) **32 Hours**

Unit 1

Electrogravimetry- coulometry- constant current and constant potential coulometry-applications-primary and secondary coulometry – conductance measurement – conductometric titrations. Ion-selective electrodes, ion-selective FET, immobilized enzyme electrodes construction.

Unit 2

Polarography – current – voltage curve. DME-components of polarographic current – supporting electrolyte – polarographic maxima. Half-wave potential-Instrumentation-Applications of Polarography. Pulse and differential pulse polarography- -stripping analysis. Amperometric titrations – Different types. Applications. Cyclic voltrametry-Theory and applications

Unit 3

Flame Emission and Atomic Absorption Spectrometer. Instrumentation of AAS, the flame spectra, flame characteristics. Atomizers used in spectroscopy, Hollow cathode lamp _ Interference in AAS-applications. Advantages of AAS over AES Atomic emission spectroscopy-flame photometry-ICP - Theory, Instrumentation and Applications.

Unit 4

Fluorescence Spectroscopy- Molecular fluorescence and fluorometers: photoluminiscence and concentration – electron transition in photoluminescence – Quenching – Fluorescence Sensors -Instrumentation for Fluorescence Spectroscopy

Unit 5

Chemical Analysis of surfaces: Surface preparations-ion scattering spectrometry secondary ion scattering microscopy (SIMS)-Auger election spectroscopy-ESCA instrumentation and application.

Principles and Applications of SEM, TEM and AFM.

References:

1. D.A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, Fundamentals of Analytical Chemistry, 8th Edn., Saunders College Pub., 2007
2. J.R.Lakowicz, Principles of Fluorescence Spectroscopy, 3rd Edn. Springer 2006
3. Analytical Chemistry, Gary D Christian, John Wiley & Sons, 2007, 6th edition
4. Principles of Analytical Chemistry, Miguel Valcarcel Cases, Springer, 2000
5. Analytical Chemistry, Jean- Michel Mermet, Matthias Otto, Robert Kellner Wiley-VCH, 2004
6. Handbook of Analytical Techniques, Volume 2, Helmut Gunzler, Alex Williams. Wiley-VCH,2001
7. Analytical chemistry, Seamus Higson, OUP Oxford, 2003
8. Reference Materials in Analytical Chemistry, Adolf Zschunke, Springer, 2000

CORE

CHE 2302 Inorganic Chemistry-III

(3 Credit) **48 Hours**

Unit 1

Compounds with transition metal to carbon bonds: classification of ligands, nomenclature, eighteen electron rule; transition metal carbonyls: Metal nitrosyls,cyanides and isocyanides. structure, bonding, spectra, preparation and reactions; transition metal organometallics. Transition metal clusters. Parallels with nonmetal chemistry isolobal analogy.

Unit 2

Metal alkyls, carbenesand carbines Nonaromatic alkene and alkyne complexes allyl and pentadienyl complexes metallocenes structure of cyclopentadienyl compounds arene complexes, complexes of cycloheptatriene,cyclooctatetraene and cyclobutadiene complexes metal clusters Application of Wade-Mingos-Lauher rules in predicting the structure of organometallic clusters and Jemmis mno rules in predicting the stability of macropolyhedral clusters

Unit 3

Homogeneous catalysis using organometallic compounds: Reactions of organometallic complexes Ligand cone angle oxidative addition, reductive elimination, insertion, nucleophilic and electrophilic attack of coordinated ligands olefin hydrogenation, hydroformylation, Wacker process, Ziegler-Natta polymerisation, cyclo oligomerisation, olefin isomerisation, olefin metathesis, Monsanto acetic acid synthesis, Fischer-Tropsch process, hydrosilylation.

Unit 4

Metal ions in biological systems: heme proteins, hemoglobin, myoglobin, hemerythrin, hemocyanin, ferritin, transferrin, cytochromes and vitamin B12; Iron-sulphur proteins: rubredoxin, ferredoxin and model systems. Copper enzymes, superoxide dismutase, cytochrome oxidase and ceruloplasmin; Coenzymes;
Molybdenum enzyme: xanthine oxidase; Zinc enzymes: carbonic anhydrase, carboxy peptidase
and interchangeability of zinc and cobalt in enzymes; Vitamin B12 and B12 coenzymes; Iron storage, transport, biomineralization and siderophores, ferritin and transferrins.

Unit 5

Applied bioinorganic chemistry, anti-cancer agents–cisplatin, radiopharmaceuticals (Tc), diagnostic (Gd in MRI) and therapeutic agents. Boron neutron capture therapy of cancer.

References:

1. B.D. Gupta and A.J. Elias "Basic Organometallic Chemistry", University Press,2010
2. P. Powell, Principles of Organometallic Chemistry, 2nd Ed., ELBS, 1991
3. I. Bertini, H. B. Gray, S. J. Lippard and J. S. Valentine, Bioinorganic Chemistry,Viva Books
4. R. W. Hay, Bio Inorganic Chemistry, Ellis Horwood, 1987.
5. J.E. Huheey, Ellen A. Keiter and Richard L. Keiter "Inorganic Chemistry, Principles of structure and Reactivity", 4th Ed., Harper Collin College Publishers, 1993
6. J. A. Cowan, Inorganic Biochemistry - An Introduction, VCH..
7. Narayan S. Hosmane (Ed) Boron Science: New Technologies and Applications, CRC Press, 2011
8. S. J. Lippard & J. M. Berg. Principles of Bioorganic Chemistry, Panima Publ. Corpn. (2005).
9. E.-I. Ochiai. Bioinorganic Chemistry – An Introduction, Allyn and Bacon Inc. (1977).
10. M. N. Hughes. The Inorganic Chemistry of Biological Processes, Wiley (1981).
11. N. Kaim & B. Schwederski. Bioinorganic Chemistry: Inorganic Elements in the Chenistry of Life, John Wiley (1994).

CORE

CHE 2303 Organic Chemistry III

(3 Credit) **48 hours**

Unit 1 (8 hours)

Nomenclature and general characteristics of heterocyclic compounds, Study of three and four-membered ring heterocyles containing one heteroatom.

Unit 2 (10 hours)

Heteroaromatic compounds (five and six-membered rings) containing one or two heteroatoms. Fused ring compounds: indole, quinoline, isoquinoline, coumarin, flavone, purine and pyrimidine bases present in nucleosides.

Unit 3 (10 hours)

Terpenoids: classification, biosynthesis; structure elucidation and synthesis of abietic acid; Steroids: classification, biosynthesis, structure of cholesterol, conversion of cholesterol to progesterone, androsterone and testosterone. Fattyacids, biosynthesis. Prostaglandins classification, structure, biosynthesis and synthesis.

Alkaloids - classification, isolation, structure elucidation based on degradative reactions (quinine and atropine). Biosynthesis of quinine and papaverine.

Unit 4 (10 hours)

Carbohydrates: Structure of ribose, glucose, fructose, maltose, sucrose, lactose, starch cellulose and cyclodextrins, Preparation of alditols, glycosides (O, C, and N), deoxysugars. Synthesis of Vitamin C from glucose. Structure and synthesis of nucleic acids, genetic code, Recombinant DNA, biosynthesis of shikimic acid.

Unit 5 (10 hours)

Aminoacids, peptides and enzymes: Synthesis of aminoacids - Strecker and azalactone synthesis, enantioselective synthesis of aminoacids, reactions of aminoacids. Structure of proteins, introduction to enzymes and coenzymes with special reference to the function of chymotrypsin, NAD, thiamine, pyridoxal. In vitro and in vivo synthesis of peptides, solid phase synthesis.

References:

1. M. Smith: Organic Synthesis, McGraw-Hill.
2. F. A. Carey and R. J. Sundberg: Advanced Organic Chemistry (part B), 3rd ed., Plenum Press.
3. T.W. G. Solomons: Fundamentals of Organic Chemistry, 5th ed., John Wiley
4. H. O. House: Modern Synthetic Reactions, W. A. Benjamin
5. W. Carruthers: Some Modern Methods of Organic Synthesis, Cambridge University Press.
6. L. Finar: Organic Chemistry Volumes 1 (6th ed.) and 2 (5th ed.), Longman.
7. J. Clayden, N. Green, S. Warren and P. Wothers: Organic Chemistry, Oxford University Press
8. N. R. Krishnaswamy: Chemistry of Natural Products; A Unified Approach, Universities Press
9. R. J. Simmonds: Chemistry of Biomolecules: An Introduction, RSC
10. R. O. C. Norman: Principles of Organic Synthesis, 2nd ed., Chapman and Hall
11. J. A. Joule, K. Mills, Heterocyclic Chemistry, 5th ed., Wiley

CORE

CHE 2304 Physical Chemistry III

(3 Credit) **48 Hours**

Unit 1 Chemical Kinetics 1

Reaction rates and order of reactions, determination of order of reactions, complex reactions, reversible, consecutive and concurrent reactions. Reactions of variable order- steady state treatment, free radical reactions-the Rice Herzfeld Mechanism. Fast reactions and relaxation methods. The reaction mechanism and molecularity. Theories of unimolecular reaction and termolecular reaction.

Unit 2 Chemical Kinetics 2

Reaction Dynamics. Theories of reaction rates. Arrhenius equation, Collision cross section and reaction cross section. Collision theory. Potential energy surfaces and reaction coordinate. Transition state theory. Comparative study of the theories of reaction rates. Thermodynamic treatment of Reaction rates.

Molecular beam methods : determination of reaction cross section.stripping and rebound mechanism. Introduction to femtochemistry.

Kinetics of reactions in solution. Diffusion controlled reactions, Effect of solvent on rates of reactions, lonic reactions and effect of ionic strength. Effect of pressure on velocity of gas reactions.

Unit 3 Chemical Kinetics 3

Catalysis and inhibition, Homogeneous catalysis, acid base and enzyme catalysis. Heterogeneous Catalysis. Mechanism of heterogeneous catalysis. Eley-Rideal and Hinshelwood mechanisms. Photochemical reaction kinetics; steady state treatment of photochemical reactions, H2 - Br2 and H2 - Cl2 reactions. Quantum yield. Quenching of fluorescence, Stern - Volmer equation. Oscillating chemical reactions. Semenoff Hinshelwood theory of chain reactions and explosions.

Unit 4 Surface Chemistry 1

Different types of interfaces- surface tension of solutions, surface excess. Thermodynamics of surfaces. The Gibbs equation and its derivation. Surface films. Surface pressure and surface potential. Lippmann equation

Adsorption by solids. The Langmuir isotherm its kinetic and statistical derivation. The Freundlich equation (no derivation). Adsorption from solution

Unit 5 Surface chemistry 2

Multilayer adsorption- the BET isotherm-its kinetic derivation. Measurement of surface area, Heat of adsoption and its determination.

Colloids, their preparation and purification, stability of colloids, Zeta potential and its determination-electrokinetic phenomena Electrophoresis, Electroosmosis, Sedimentation and streaming potential ; Donnan membrane equilibrium and its applications

Unit 6 Surface chemistry 3

Colloidal Surfactants, Micelles, HLB number. Stabilising action of surfactants, Practical importance of surfactants. Langmuir- Blodget films. Morphological studies. Sol –gel process- preparation of ordered microporous and mesoporous materials by sol-gel process. Preparation of pyrovskites and spinels by Sol-gel process. Sol-gel process and nanomaterials.

References:

1. W. J. Moore and R. G. Pearson, Kinetics and Mechanism, Wiley, New York, 1988
2. K. J. Laiddler, Chemical-Kinetics, McGraw Hill, New York, 1991.
3. F. Daniels and R. A. Alberty, Physical Chemistry, 8h Edition, Wiley, New York, 1994
4. P. W. Atkins, Physical Chemistry 8th Edn., Wiley, New York, 2006
5. A. W. Adamson, The Physical Chemistry of Surfaces, 2nd Edn., Wiley. New York, 1998

6. A. Somorjai, Chemistry of Surfaces, 3rd Edn. Wiley, New York, 2005
7. A. Alexander and P. Johnson, Colloid Science, Oxford University Press, Oxford, New York, 1996.

CHE 2305 PHYSICAL CHEMISTRY LAB

(2 Credit) 80 hours

1. Molecular weight determination by cryoscopic methods, Formula of complexes.

2. Phase diagrams : Two component liquid–liquid and solid-liquid systems. Three component liquid-liquid systems.

3 Determination of transition temperature, molecular` weight determination.

4. Refractometry : Variation of refractive index with composition, formula of complexes.

5. Chemical Kinetics : Acid and base catalysed hydrolysis of esters, Dependence of temperature and ionic strength on the rate of reactions.

6. Specific rotation of cane sugar and inversion of cane sugar by acid.

7. Ostwald Viscometer: Viscosity of liquid and liquid mixtures.

8. Conductometry : Cell constant, conductivity of a weak-acid, solubility of a sparingly soluble salt, conductometric titrations.

9. Poteniometry : Measurement of electrod potentials, activity coefficients and potentiometric titrations , pH metric titations.
10. Spectrophotometry
11. Flamephotometry
12. AAS

1. A.Findlay, Practical Physical Chemistry, Longman
2. F.Daniels et al Experimental Physical Chemistry, McGraw Hill
3. Shoemaker, Garlands “Experimentals in Physical Chemistry” McGraw Hill

ELECTIVE

CHE 2306 SOLID STATE CHEMISTRY

(2 Credit) **32 Hours**

Unit 1

Band theory of solids- energy bands, conductors and non-conductors, intrinsic semiconductors, extrinsic semiconductors, Hall effect.

Unit 2

Stoichiometric Defects: Equilibrium concentration of point defects in crystals - Schottky defects, Frenkel defects; The photographic process - light sensitive crystals, mechanism of latent imageformation, lithium iodide battery.Non-Stoichiometric Defects: Origin of non-stoichiometry, consequences of non-stoichiometry; Equilibria in non-stoichiometric solids, Color centers: F-centre, electron and hole centre; colour centre and information storage.

Unit 3

Electrical properties; conductivity in pure metals; superconductivity; basics, discovery and high Tc superconductors magnetic properties; ferromagnetic and antiferromagnetic materials

Unit 4

Optical properties; photoconductivity, photovoltaic effect, applications, luminescence. Electrical properties: dielectric properties, piezo-electricity, Ferro electricity. Lasers and their applications in chemistry.

Unit 5

Preparative methods: Solid state reaction, chemical precursor method, co-Precipitation, sol-gel, metathesis, self-propagating high temperature synthesis, ion exchange reactions, intercalation/deintercalation reactions; hydrothermal and template synthesis; , preparation of thin films - electrochemical methods, chemical vapour deposition; Crystal growth - Bridgman & Stokbarger methods, zone melting.
Characterization of Solids: Crystal growing; Data collection, data reduction, refinement and structure solution of some compounds

References:

1. R. West. Solid State Chemistry and its Applications, John Wiley (1987).
2. N. B. Hannay, Solid State Chemistry, Prentice Hall of India (1979)
3. R. J. D. Tiley. Defect Crystal Chemistry and its Applications, Chapman and Hall, NewYork (1987).
4. L.V. Azaroff "Introduction to Solids" Mc.Graw Hill, New York, 1960.
5. A.K. Galwey, Chemistry of Solids, Chapman and Hall, London, 1967.
6. Lesley Smart and Elaine Moore, Solid State Chemistry, Chapman and Hall, 1995.
7. H. V. Keer, Principles of the Solid State Wiley Eastern Ltd, New Delhi, 1993.

ELECTIVE

CHE 2307 Industrial Catalysis

(2 Credit) **32 Hours**

Unit 1

Adsorption and catalysis – adsorption and reaction rate – strength of adsorption bond and catalysis – adsorption equilibrium and catalysis, kinetics of heterogeneous catalysis: diffusion steps neglected – unimolecular reactions – bimolecular reactions – Langmuir-Hinshelwood and Eley-Rideal mechanism, kinetics of heterogeneous catalysis: diffusion controlling – mechanism of diffusion – diffusion and reaction

in pores – selectivity and diffusion, electronic factors in catalysis by metals, electronic factors in catalysis by semiconductors, geometric factors and catalysis.

Unit 2

Surface area and porosity measurement – measurement of acidity of surfaces; Support materials – preparation and structure of supports – surface properties, preparation of catalysts – introduction of precursor compound – pre-activation treatment – activation process. General methods of synthesis of zeolites, mechanism of nuclear formation and crystal growth, structures of some selected zeolites – zeolites A, X and Y, pentasils – ZSM-5, ZSM-11, shape selective catalysis by zeolites.

Unit 3

Deactivation of catalysts, classification of catalyst deactivation processes, poisoning of catalysts, coke formation on catalysts, metal deposition on catalysts, sintering of catalysts, Regeneration of deactivated catalysts, feasibility of regeneration, description of coke deposit and kinetics of regeneration.
Basic concepts in phase transfer catalysis – phase transfer catalyzed reactions – basic steps of phase transfer catalysis – effect of reaction variables on transfer and intrinsic rates – outline of compounds used as phase transfer catalysts

Unit 4

Enzymes – an introduction to enzymes – enzymes as proteins – classification and nomenclature of enzymes – structure of enzymes – how enzymes work – effect on reaction rate – thermodynamic definitions – catalytic power and specificity of enzymes – optimization of weak interactions between enzyme and substrate in the transition state – binding energy, reaction specificity and catalysis – specific catalytic groups contributing to catalysis.

Unit 5

Oil based chemistry; catalytic reforming; catalytic cracking; paraffin cracking; naphthenic cracking; aromatic hydrocarbon cracking; isomerization; hydrotreatment; hydrodesulphurization; hydrocracking; steam cracking; hydrocarbons from synthesis gas; Fisher-Tropsch process, Mobil process for conversion of methanol to gasoline hydrocarbons. Catalysis for environmental protection, removal of pollutants from exhausts, mobile and static sources.

References:

1. R.J. Farrauto and C.H. Bartholomew, “Fundamentals of Industrial Catalytic Processes”, Blackie Academic and Professional – Chapman and Hall, 1997.
2. R. Pearce and W.R. Patterson, “Catalysis and chemical processes”, Academic press, Leonard Hill, London, 1981.
3. Clark, “Theory of adsorption and catalysis”, Academic Press, 1970.
4. J.M. Thomas & W.J. Thomas, “Introduction to principles of heterogeneous catalysis”, Academic Press, New York, 1967.
5. R.H.P. Gasser, “An introduction to chemisorption and catalysis by metals”, Oxford, 1985.
6. D.K Chakraborthy, “Adsorption and catalysis by solids”, Wiley Eastern Ltd. 1990.
7. J.R. Anderson and M. Boudart (Eds), “Catalysis, Science and Technology”, Vol 6, Springer-Verlag, Berlin Heildberg, 1984.
8. R. Szostak, “Molecular sieves: principles of synthesis and identification”, Van Nostrand, NY, 1989.
9. R. Hughes, “Deactivation of catalysts”, Academic press, London, 1984.

10. C.M. Starks, C.L. Liotta and M. Halpern, "Phase Transfer Catalysis – fundamentals, applications and industrial perspectives", Chapman & Hall, New York, 1994.
11. A.L. Lehninger, "Principles of Biochemistry", Worth Publishers, USA, 1987.

ELECTIVE

CHE 2308 MICROBIAL TECHNOLOGY

(2 Credit) **32 Hours**

Unit 1

Industrial microorganisms: differentiation between prokaryotes and eukaryotes; General characteristic, structures, nutrition, growth, reproduction and economic importance of bacteria, Economic importance of fungi and acinomycets

Prevention and control of microorganisms- Control by physical and chemical agents-

Unit 2

Fermentation techniques: Screening procedures; preservation and maintenance of industrial microorganisms; batch, fed batch and continuous fermentation. Fermentor.

Down stream processing- Introduction, separation- filtration, centrifugation, flocculation and flotation; disintegration of cells-mechanical and nonmechanical methods; extraction. Concentration methods- evaporation, membrane filtration, ion exchange. Purification- chromatography, drying and crystallization.

Unit 3

Manufacture of Beer, Production of alcohol by fermentation.

Manufacture of diary products- Butter, Cheese. Fermented milk beverages- kefir, kumiss. Yoghurt. Microbial production of antibiotic- Penicillin, streptomycin.

Unit 4

Microbial production of Organic acids and Amino- Citric and acetic acid; glutamic acid, lysine. Microbial production of vitamins- vitamin B12 and Riboflavin

Microbial transformation of steroid and sterol.

Unit 5

Production and purification of microbial enzymes- protease, amylases, lipases and their industrial application. Enzyme immobilization- various methods of immobilization and application of immobilized enzymes.

References:

1) P F. Stanbury, A Y Whitaker and S J Hall, "Principle of Fermentation Technology Elsiever, 2003, online published 2007
2) Pelzar, Reid and Chan, "Microbiology" McGraw Hills inc., New York, 1979
3) Casida L.E, Industrial Microbiology, 1984
4) Peppler and Pearlman, Microbial Technology, Academic press, 1979
5) John B'uock and Bjorn Kristansen, Basic Biotechnology, Academic Press, 1987.

ELECTIVE

CHE 2309 Advanced Photochemistry

(2 Credit) **32 Hours**

Unit 1

Energy Transfer-Theories of Energy Transfer – Photosensitization of Organic and Inorganic Molecules – Singlet Oxygen – Methods of singlet oxygen generation and Detection – Chemistry of Singlet Oxygen – Photodynamic Therapy of Cancer

Unit 2

Photoinduced Electron Transfer – Theory of Electron transfer – Circumventing Back Electron transfer – Photoinduced Electron transfer reactions of Organic and Inorganic Molecules – Photosynthesis – Artificial Solar Energy Harvesting – Photochemical Splitting of Water – Dye – sensitized solar cells - Grätzel Cell - Bulk heterojunction devices for solar energy harvesting - Organic light emitting devices.

Unit 3

Photochemistry and Photophysics of Semiconductors – Semiconductor Photocatalysis - Photochemistry and Advanced Materials - Photoresists – Photolithography – Photochromism – Photonic Materials and Lasers

Unit 4

Photochemistry in Practice – Radiometry and Actinometry – Priciples of Radiometry and radiometers – Actinometry – Quantum Yields – Light Sources – Optical Materials and Filters – Photochemical Reactors

References:

1. Modern Molecular Photochemistry, Nicholas J. Turro, University Science Books; New Ed edition
2. Photochemistry (Oxford Chemistry Primers), Carol E. Wayne, Oxford University Press; 1 edition (1996)
3. Principles of Fluorescene Spectroscopy, Joseph R. Lakowicz, Plenum Press, 3rd edition
4. Photochemical Technology, Andre M. Braun, Marie-Therese Maurette, Esther Oliveros, John Wiley & Sons
5. Photoinduced Electron Transfer by Marye Anne Fox and M. Chanon Part A, B. C and D, Elsevier Science Publishing Company
6. Photoinduced Electron Transfer 1-5 (Topics in Current Chemistry) by J.,Ed. Mattay, Springer; 1 edition
7. Fundamentals of Photoinduced Electron Transfer by G. J. Kavarnos, Wiley-VCH; 1 edition
8. Semiconductor Photochemistry and Photophysics (Molecular and Supramolecular Photochemistry), V. Ramamurthy, Marcel Dekker; 1 edition

ELECTIVE

CHE 2310 Introduction to Computational Chemistry

(2 Credit) **32 hours**

Unit 1

Tools and philosophy of computational chemistry. Fundamental molecular forces-the dynamic equation – solving dynamic equation. Separation of variables- separating time and space variables – separating nuclear

and electronic variables. Separation of variables and hybrid modeling. Quantum chemical description of the system – hydrogen and helium atoms. Many electron wave functions- second quantization. Reduced density matrices- Resolvents and Green's functions. Potential energy surfaces-Born – Oppenheimer approximation-geometry optimization- stationary points

Unit 2

Molecular mechanics and force fields-the force field energy. Force field parameterization- parameter reductions- universal force fields Transferability of force fields. Calculation of energy and geometry of molecules- treatment of delocalized pi-systems- coordinate space for geometry optimization-optimization algorithm. Hybrid MM methods-mechanical embedding- IMOMM, IMOMO, ONIOM. Polarization embedding. Deductive Molecular mechanics – bridging with quantum chemical methods. Stereochemistry and VSPER theory

Unit 3

Methods of molecular structure- Hybrid perspective.– pseudo potential and valence approximation. Hartree-Fock approximation- HF-Roothaan's theorem and semi empirical methods- all valence semi empirical methods- pi- approximation. Non HF- R semi empirical methods- linear scaling semi empirical methods for organic molecules – SLG approximation- semiemperical methods for transition metal complexes. Effective Hamiltonian for the crystal field

Unit 4

Electronic structure methods-independent particle models- SCF methods- energy of a Slater determinant-Koopman's theorem. The Basis set approximation- Restricted and unrestricted Hartree Fock- NDDO, INDO, CNDO methods. Parameterization- MINDO, AM1, PM3. Extended Huckel theory. PM. Electron correlation – excited Slater determinants- configuration interaction. The UHF dissociation and the spin contamination problem. Many body perturbation theory- Moller-Plesset perturbation theory. Coupled Cluster theory. Basis sets- Slater and Gaussian type orbitals. Even and well tempered Basis sets. Contracted Basis sets. Construction of the Z- matrix

Unit 5

Density Functional methods- orbital free DFT. Kohn – Sham theory (LCAO equations). Reduced density matrix methods. Exchange and correlation holes. Exchange- correlation functional. Linear scaling techniques. Pauli and Thomas – Fermi models. Hohenberg- Kohn theorems. Numerical integration (Quadrature). Custom and Hybrid functional. Local density approximations. Beyond the local density approximation. The Becke exchange correction . The Lee-Yang – Paar Correlation Potential

Unit 6

Determination of molecular properties using molecular mechanics, ab initio, semi empirical and DFT methods. Wave function analysis- population analysis. Geometry, Total energy, Dipole moment, vibrational frequency, Chemical Shifts. Determination of orbital energy gap – electronic spectral transitions. Application to polymers- periodic boundary condition. Determination of polarizability and hyperpolarizability of organic molecules and polymers. Interaction with solvents and solvent effects- Onsager model. Solvatochromism.

Reference:

1. F. Jensen, Introduction to Computational Chemistry, 2nd Edn., Wiley, New York, 2009
2. A. R. Leach, Molecular Modeling, Principles and Applications,2nd Edn., Pearson Education, London, 2001

3. A. Hinchliffe, Modeling Molecular Structures, 2nd Edn., Wiley, New York, 2000
4. D. Young, Computational Chemistry: A Practical Guide to Real World Problems, Wiley, New York, 2001
5. A. L. TCHOUGRÉEFF, Hybrid Methods of Molecular Modeling, Springer, Berlin, 2008
6. A. Hinchliffe, Molecular Modeling for Beginners, 2nd Edn., Wiley, New York, 2008
7. A. Haaland, Molecules and Models: The Molecular Structures of Main Group Element Compounds, Oxford University Press, Oxford, New York, 2008
8. E. Lewars, Computational Chemistry. Introduction to the Theory and Applications of Molecular and Quantum Mechanics, Kluwer Academic, New York, 2004

CHE 2401 Project Dissertation (16 Credit)
CHE 2402 Viva Voce