COCHIN UNIVERSITY OF SCIENCE AND TECHNOLOGY

DEPARTMENT OF APPLIED CHEMISTRY

SYLLABUS FOR M.Sc. CHEMISTRY
(*WITH EFFECT FROM 2019-20*)

DEPARTMENT OF APPLIED CHEMISTRY

M.Sc. CHEMISTRY

COURSE STRUCTURE AND SYLLABUS

(WEF 2019-20)

SEMESTER I

Course	Core/ Elective	Credits	Marks		Total Marks
			Internal	External	
CHE 2101 Inorganic Chemistry -I *(Main Group Elements)*	Core	3	50	50	100
CHE 2102 Organic Chemistry-I (*Structure and Reactivity*)	Core	3	50	50	100
CHE 2103 Physical Chemistry-I *(Quantum Chemistry and Chemical Bonding)*	Core	3	50	50	100
CHE 2104 Group Theory and Spectroscopy	Core	3	50	50	100
CHE 2105 Inorganic Chemistry Lab	Core	2	100		100
CHE 2106 Equilibrium and Nonequilibrium Thermodynamics	Elective	3	50	50	100
CHE 2107 Environmental Chemistry	Elective	2	50	50	100
CHE 2108 Chemistry of Polymers	Elective	2	50	50	100
CHE 2109 Spectroscopic Techniques	Interdepartmental Elective	2	50	50	100

<u>**SEMESTER II**</u>

Course	Core/ Elective	Credits	Marks		Total Marks
			Internal	External	
CHE 2201 Analytical Chemistry	Core	2	50	50	100
CHE 2202 Inorganic Chemistry-II *(Chemistry of d- and f-block Elements)*	Core	3	50	50	100
CHE 2203 Organic Chemistry- II *(Reactions and Mechanisms)*	Core	2	50	50	100
CHE 2204 Organic Chemistry-III *(Reagents and Synthesis)*	Core	2	50	50	100
CHE 2205 Physical Chemistry- II *(Statistical Thermodynamics and Electrochemistry)*	Core	3	50	50	100
CHE 2206 Organic Spectroscopy	Core	2	50	50	50
CHE 2207 Organic Chemistry Lab	Core	2	100	-	100
CHE 2208 Introduction to Theory of Orbital Interactions in Chemistry	Elective	2	50	50	100
CHE 2209 Introduction to Materials Chemistry	Elective	2	50	50	100
CHE 2210 Stereoselective Synthesis	Elective	2	50	50	100
CHE 2211 Polymer Technology	Elective	2	50	50	100
CHE 2212 Bioanalytical Chemistry	Elective	2	50	50	100
CHE 2213 Advanced Photochemistry	Elective	2	50	50	100
CHE 2214 Chemical Instrumentation	Interdepartmental Elective	2	50	50	100

SEMESTER III

Course	Core/ Elective	Credits	Marks		Total Marks
			Internal	External	
CHE 2301 Instrumental Methods of Analysis	Core	2	50	50	100
CHE 2302 Inorganic Chemistry- III *(Organometallic and Bioinorganic Chemistry)*	Core	3	50	50	100
CHE 2303 Organic Chemistry-IV *(Natural Products)*	Core	4	50	50	100
CHE 2304 Physical Chemistry-III *(Kinetics, Surface Chemistry and Catalysis)*	Core	3	50	50	100
CHE 2305 Physical Chemistry Lab	Core	2	100	-	100
CHE 2306 Nuclear and Radiation Chemistry	Elective	3	50	50	100
CHE 2307 Industrial Catalysis	Elective	3	50	50	100
CHE 2308 Medicinal Chemistry	Elective	4	50	50	100
CHE 2309 Solid State Chemistry and Crystallography	Elective	4	50	50	100
CHE 2310 Molecular Modeling in Chemistry	Elective	4	50	50	100
CHE 2311 Microbial Technology	Elective	2	50	50	100
CHE 2312 Chemistry of Carbohydrates	Elective	2	50	50	100

SEMESTER IV

Course	Core/ Elective	Credits	Marks		Total Marks
			Continuous Evaluation	End Sem	
CHE 2401 Dissertation	Core	16	150	150	300

CORE

CHE 2101 Inorganic Chemistry - I

(Main Group Elements)

(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; electron counting in polycondensed polyhedral boranes, mno rule. 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, M. Bochmann, Advanced Inorganic Chemistry, 6^{th} ed., Wiley-Interscience: New York, 1999.
2. E. Huheey, E. A. Keiter, R. L. Keiter, Inorganic Chemistry: Principles of Structure and Reactivity, 4^{th} ed., Harper Collin College Publishers, 1993.
3. J. W. Steed, J. L. Atwood, Supramolecular Chemistry, 2^{nd} ed., John Wiley and Sons Ltd., 2009.
4. D. F. Shriver, P. W. Atkins, C. H. Langford, Inorganic Chemistry, 3^{rd} ed., ELBS, 1999.
5. B. Douglas, D. McDaniel, J. Alexander, Concepts and Models of Inorganic Chemistry, 3^{rd} ed., Wiley.
6. N. N. Greenwood, A. Earnshaw, Chemistry of the Elements, 2^{nd} ed., BH, 1997.

CORE

CHE 2102 Organic Chemistry -I

(Structure and Reactivity)

(3 Credit) **48 Hours**

Unit 1

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

Geometrical isomerism, origin – structural features including C-C and C-hetero atom double bonds, cyclic systems and other systems exhibiting restricted rotation, different nomenclature including, cis-tarns, E-Z, syn-anti, endo-exo, in-out, relative acidity of maleic and fumaric acids

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.

Conformational analysis, Acyclic sp^3–sp^3, sp^3-sp^2 systems, structure and stability of small, medium, and large rings, cyclohexane, substituted cyclohexanes, A values, cyclohexenes, decalins, bicyclic systems. Strain, types of strain including B, F, I, Pitzer strain, Beyer strain.

Unit 3

Classification of reactions according to IUPAC conventions. Reaction mechanism: guidelines on Pushing of electrons. Reactive intermediates: Formation, stability and general reactivity. 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. Carbon acids: pK_a of weak acids, 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

Frontier Orbitals, HSAB concept, Perturbation theory of reactivity. 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.

Unit 5

Pericyclic reactions, study of the principle of conservation of orbital symmetry: Orbital symmetry diagrams for cycloaddition and electrocyclic reactions, Study of Frontier Molecular Orbital Theory, Aromatic Transition State Theory and The Generalized Woodward – Hoffmann rule applied to cycloaddtions, Electrocyclic reactions, Sigmatropic rearrangements and Chelotropic reactions– Stereochemistry and Regiochemistry of Cycloaddtions. Substituent and medium effects, Secondary Orbital Interactions in [4+2] cycloadditions, Intramolecular Diels–Alder reactions. 1,3-dipolar cycloaddition reactions. Photochromism and thermochromism, Cope rearrangement, Claisen rearrangement and ene-reaction.

References:

1. J. March, Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 7th ed. Wiley, 2013.
2. T. H.Lowry, K.S.Richardson, Mechanism and Theory in Organic Chemistry, 3rd ed., Benjamin-Cummings Publishing Company,1997.
3. F. A. Carey, R. J. Sundberg, Advanced Organic Chemistry (parts A and B), 5th ed., Springer, 2008.
4. E. V. Anslyn, D. A. Dougherty, Modern Physical Organic Chemistry. University Science Books, 2006.
5. F. A. Carroll, Perspectives on structure and mechanism in organic chemistry, Wiley, 2011.
6. N. S. Issacs, Physical Organic Chemistry, 2nd Edition, Prentice Hall, 1995.
7. A. Pross, Theoretical and Physical Principles of Organic Chemistry, 1st ed., Wiley, 1995.
8. J. Clayden, N. Green, S. Warren, P. Wothers, Organic Chemistry, 2nd ed., Oxford University Press, 2012.
9. I. Flemming, Frontier orbitals and organic chemical reactions, Wiley-Blackwell, 1976.
10. I. Flemming: Molecular orbitals and organic chemical reactions, student ed., Wiley, 2009.
11. J. McMurry, Organic Chemistry, 5th ed., Brooks/Cole, 2000.
12. R. Bruckner, Advanced organic chemistry: Reaction Mechanisms. Academic Press, 2001.
13. P.S.Kalsi, Stereochemistry, Conformation and Mechanism, 3rd ed., New Age Publications.
14. E. L. Eliel, S. H. Wilen, Stereochemistry in Organic Compounds, John Wiley, 1994.
15. D. Nasipuri, Stereochemistry of Organic Compounds: Principles and Applications, 2nd ed., Wiley Eastern Limited, New Delhi, 1994.

CORE

CHE 2103 Physical Chemistry - I

(Quantum Chemistry and Chemical Bonding)

(3 Credit) **48 Hours**

Unit 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, Vibrational motion, Harmonic oscillator, Method of power series, Hermite equation and Hermite Polynomials, Recursion formula, Rodrigues formula, wave function and energy.

Unit 2

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 L^2 and L_z, 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. Postulate of electron spin - orbital and spin functions. Many electron atoms.

Unit 3

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, The Coulomb and Exchange Operators, The Fock Operator, Koopmans' theorem, Brillouin's theorem, The Roothaan Equations, Slater's treatment of complex atoms, Slater orbitals. Pauli principle, Slater determinant and wave function.

Unit 4

Chemical boning, Born Oppenheimer approximation, Valence bond method. Comparison of VB and MO method, Bonding in simple molecules like water, BF_3, NH_3, CH_4, VSEPR theory, Molecular orbital method for homo and hetero diatomic molecules. Pi bonding in simple molecules, HMO method for linear conjugated hydrocarbons, ethylene, 1,3-butadiene, allyl radical, cation and anion, aromatic hydrocarbons, cyclopropenyl systems, cyclobutadiene, benzene, calculation of free valence charge density and reactivity.

Unit 5

Fragment molecular orbitals of CH, CH_2 and CH_3, Molecular orbital construction from fragment orbitals. Walsh diagram, Molecular orbital of small molecules like methane, ethane, propane, methyl halides, formaldehyde and reactive intermediates carbocations, carbanions, radicals, pi-bonding effect of ligand, Correlation diagram, Non-crossing rule. Orbital interactions through space and through bonds.

References:

1. N. Levine, Quantum Chemistry, 6^{th} ed., Pearson Education, London, 2008.
2. D. A. McQuarrie, Quantum Chemistry, 3^{rd} ed., Univ. Sci. Books, Mill Valley, California, 1983.
3. J. P. Lowe, Quantum Chemistry 3^{rd} ed., Academic Press, New York, 2008.
4. P. W. Atkins, R.S Friedman, Molecular Quantum Mechanics, 5^{th} ed., OUP, Oxford, 2012.
5. P.W. Atkins, Physical Chemistry, 8^{th} ed., Wiley, New York, 2006.
6. L. Pauling, E. B. Wilson Jr., Introduction to Quantum Mechanics with Applications to Chemistry, Dover Book ed., Mc.Graw-Hill, New York, 1935.
7. A.Szabo, N. S. Ostlund, Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory, Dover Book ed., Mc.Graw-Hill, New York, 1982.
8. T. A. Albright, J. K. Burdett, M.-H. Whangbo, Orbital Interactions in Chemistry, 2^{nd} ed., John Wiley and Sons, Inc., Hoboken, New Jersey, 2013.
9. I. Flemming, Frontier Orbitals and Organic Chemical Reactions, Wiley-Blackwell, 1976.
10. I Flemming, Molecular Orbitals and Organic Chemical Reactions, Students ed., Wiley, 2009.
11. D. D. Fitts, Principles of Quantum Mechanics as Applied to Chemistry and Chemical Physics, CUP, Cambridge, New York, 2002.
12. L. Piela, Ideas of Quantum Chemistry, Elsevier, Amsterdam, 2007.

CORE

CHE 2104 Group Theory & Spectroscopy

(3 Credit) **48 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 ed., 1992.
2. V. Ramakrishnan, M. S. Gopinathan, Group theory in Chemistry, Vishal Pub. New Delhi, 1996.
3. P. W. Atkins, Physical Chemistry 8th ed., W. H. Freeman, New York, 2006.
4. R. A. Alberty, Physical Chemistry 8th ed., 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 ed., 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, 2nd ed., Saunders College Publication, 1992.
9. D. H. Williams, I. Flemming, Spectroscopic Methods in Organic Chemistry, 4th ed., McGraw-Hill, 1985.
10. H. Gunther, NMR Spectroscopy, 2nd ed., John Wiley, 2005.
11. N. B. Colthup, L. H. Daly, S. E. Wiberley, Introduction to Infrared and Raman Spectroscopy, 3rd ed., 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 (Zn^{2+}, Mg^{2+}). 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 D_q values. Determination of crystal field splitting energy for certain ligands and construction of a part of the spectrochemical series

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 Equilibrium and Non-Equilibrium Thermodynamics

(3 Credit) **48 hours**

Unit 1

Mathematical Techniques, Variables of thermodynamics, Theoretical Methods, Practical techniques, Exact and Inexact Differentials, First law of thermodynamics, State functions, Thermodynamic Functions- Internal energy, Enthalpy, Heat capacity, Different types of processes- Reversible and Irreversible, Isothermal and Adiabatic, Joule Thomson effect, Applications, Co-efficient of thermal expansion,

Unit 2

Second law of thermodynamics. Entropy as a state function, The Clausius inequality. Entropy changes accompanying expansion, phase transition and heating. Free energy functions - Variation with temperature and pressure. Gibbs Helmholtz equation. Relation between thermo dynamic functions. Maxwell relations.

Third law of thermodynamics: Nernst Heat Theorem, Calculation of absolute entropy, Unattainability of absolute zero.

Thermodynamic systems of variable composition – Partial molar properties. Chemical Potential, Gibbs Duhem Equation and Duhem Margules Equation. Thermodynamics of mixing. Concepts of activity and fugacity, Standard states.

Thermochemistry- Standard enthalpy changes and Heat of formation, Hess's Law, Kirchoff's Law. Entropy and Gibbs energy of formation.

Unit 3

Physical transformation of Pure substances- Stability of a phase, Phase transitions and phase boundaries- Thermodynamic aspects, Ehrenfest Classification of Phase transitions. Phase rule – Application to one, two and three component systems

Solutions- Ideal solutions, Raoults law, Henry's Law, Deviations from ideality, Real and Regular solutions, Excess functions, Ideal Dilute Solutions- Colligative Properties- van't Hoff factor.

Liquid-vapour, liquid- liquid and solid-liquid equilibria of binary systems.

Unit 4

Chemical Equilibria and free energy, Equilibrium Constants, Applications of free energy function to physical and chemical charges. Effect of temperature and pressure on chemical equilibrium- van't Hoff reaction isotherm and isochore.

Unit 5

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. Biological Motors, Earths energy balance.

References:

1. P. Atkins, J. de Paula, Physical Chemistry, 7^{th} ed., W. H. Freeman and Company, New York. 2006.
2. I.M.Klotz, R.M.Robsenberg, Chemical Thermodynamics, 3^{rd} ed., A.Benjamin, INC.1972.
3. L.K.Nash, Elements of Chemical Thermodynamics, 2^{nd} ed., Addison Wesley, 2005.
4. I. Prigogine, Introduction to Thermodynamic Irreversible Processes, 3^{rd} ed., Wiley Interscience, 1968.
5. S. R. de Groot, P. Mazur, Non-equilibrium Thermodynamics, Dover Publications, 2011.
6. G. Lebon, D. Jou, J. Casas, Understanding Non-equilibrium Thermodynamics, Springer. 2008.

ELECTIVE

CHE 2107 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.

Unit 3

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. G. W. VanLoon, S. J. Duffy, Environmental Chemistry, Oxford University Press, 2005.
2. J. Girard, Principles of Environmental Chemistry, Jones & Bartlett Learning, 2005.
3. S. E. Manahan, Environmental Chemistry, 7^{th} ed., CRC Press, 2010.
4. E. R. Weiner, Applications of Environmental Chemistry, CRC Press, 2010.
5. I. Williams, Environmental Chemistry, John Wiley, 2001.
6. G. Schwedt, The Essential Guide to Environmental Chemistry, John Wiley, 2001

ELECTIVE

CHE 2108 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. Fluorine 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 ed., 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 ed., 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.

ELECTIVE (INTER DEPARTMENTAL)

CHE 2109 Spectroscopic Techniques

(2 Credit) 32 hours

Unit 1

Spectroscopy as a physical property of molecules, different regions of electromagnetic spectrum and energy associated with a particular frequency, basics of light absorption, factors affecting sensitivity, absorption characteristics, structural information based on absorption characteristics.

Unit 2

Introduction to microscopic and X-ray techniques. Confocal microscopy, fluorescence and radioisotope labeling as diagnostic tools. Basic introduction to Electron microscopy: types, sample preparation and analysis. Powder XRD and single crystal XRD.

Unit 3

UV-visible spectroscopy – allowed and forbidden transitions, chromophores, auxochromes, effect of structure on absorption characteristics, basics of ORD and CD and emission spectroscopy.

IR spectroscopy - intra and intermolecular hydrogen bonding, effect of concentration and temperature, Fourier transform IR, group frequencies, fundamental frequencies and overtones, Fermi Resonance.

Unit 4

Spectroscopy - experimental aspects, FT NMR, factors influencing sensitivity and resolution, applications of chemical shift and spin-spin coupling, analysis of spin systems, factors affecting coupling constants, NMR of carbon-13, DEPT analysis and brief introduction to correlation spectroscopy (COSY, HMBC and HSQC only). Brief introduction to NMR of other biologically relevant nuclei such as ^{15}N, ^{2}D and ^{31}P.

Unit 5

Mass spectrometry - high resolution mass spectrometry, soft ionization techniques, MS/MS data, application of GC-MS and LC-MS data, introduction to fragmentation modes and determination of primary structure of peptides on the basis of mass spectral data.

Problems based on combined application of various spectroscopic techniques to examine secondary structure of peptides, DNA melting etc.

References:

1. D.L.Pavia, G.M.Lampman, G.S.Kriz, Introduction to Spectroscopy, A Guide for Students of Organic Chemistry, 3rd ed., Thomson. 2004.
2. Atta-Ur-Rahman, M.I.Choudhary, Solving Problems with NMR Specroscopy, Academic Press, New York, 1996.
3. L. D Field, S Sternhell, J R Kalman, Organic Structures from Spectra, 4th ed., Wiley, 2008.
4. R. S. Drago, Physical Methods for Chemist, Saunders, 1992.
5. C. N. Banwell, E. M. McCash, Fundamentals of Molecular Spectroscopy, 4th ed., McGraw-Hill, 1994.
6. D.F.Taber, Organic Spectroscopic Structure Determination, A Problem Based Learning Approach, Oxford University Press, 2009.
7. H. Gunther, NMR Spectroscopy, 2nd ed., John Wiley and Sons, 1995.
8. R. M. Silverstein, G.C. Bassler, T. C. Morril, Spectroscopic identification of organic compounds, John Wiley, 1991.
9. D. H. Williams, I. Fleming, Spectroscopic Methods in Organic Chemistry, Tata McGraw Hill. 1988.
10. W. Kemp, Organic Spectroscopy, 2nd ed., ELBS-Macmillan, 1987.
11. F. Bernath, Spectra of Atoms and Molecules, 2nd ed., Oxford University Press, 2005.
12. E. B. Wilson, Jr., J. C. Decius, P. C. Cross, Molecular Vibrations: The Theory of Infrared and Raman Spectra, Dover Publications, 1980.
13. A. Weil, J. R. Bolton, Electron Paramagnetic Resonance: Elementary Theory and Practical Applications, 2nd ed., Wiley Interscience, John Wiley & Sons, Inc., 2007.
14. C. P. Slichter, Principles of Magnetic Resonance, 3rd ed., Springer-Verlag, 1990.
15. H. Gunther, NMR Sprectroscopy: Basic principles, Concepts, and Applications in Chemistry, 2nd ed., Wiley 1997.
16. Spectral data bases (RIO DB of AIST, for example)

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, 8^{th} ed., Saunders College Pub., 2007.
2. G. D Christian, Analytical Chemistry, 6^{th} ed., John Wiley & Sons, 2007.
3. M.V. Cases, Principles of Analytical Chemistry, Springer, 2000.
4. J.- M. Mermet, M. Otto, R. Kellne, Analytical Chemistry, Wiley-VCH, 2004.
5. H. Gunzler, A. Williams, Handbook of Analytical Techniques, Volume 2, Wiley-VCH, 2001.
6. S. Higson, Analytical Chemistry, OUP Oxford, 2003.
7. A. Zschunke, Reference Materials in Analytical Chemistry, Springer, 2000.

CORE

CHE 2202 Inorganic Chemistry -II

(Chemistry of d- and f-block Elements)

(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 and 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 d^7, d^5 and low spin d^6 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. 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, M. Bochmann Advanced Inorganic Chemistry, 6th ed., Wiley-Interscience: New York, 1999.
2. J.E. Huheey, E. A. Keiter, R. 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 ed., 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., John Wiley and Sons, 1994.
6. N. N. Greenwood, A. Earnshaw, Chemistry of the Elements, 2nd ed., BH, 1997.
7. R. S.Drago, Physical Methods for Chemists, 2nd ed., Saunders College Publishing, 1992.

CORE

CHE 2203 Organic Chemistry-II

(Reactions and Mechanisms)

(2 Credit) **32 Hours**

Unit 1

Aliphatic substitution reactions – saturated and unsaturated systems – Mechanism of nucleophilic substitution – S_N2, S_N1 – ion pairs, SET, Neighbouring group participation – non classical carbocations, S_Ni, Tetrahedral mechanism. Electrophilic substitution – S_E2, S_Ei, S_E1. Free radical substitution. Reactivity – Effect of substrate structure, nature of reagents, solvents and stereochemistry on the outcome of these reactions. Ambident nucleophiles and substrates. Typical reactions in organic synthesis.

Unit 2

Mechanisms of polar addition – electrophilic, nucleophilic and free radical addition. Nonpolar additions (excluding pericyclic reactions) - Reactivity and orientation. Eliminations - E2, E1 and E1CB mechanisms, reactivity and orientation. Pyrolytic syn eliminations, a - eliminations, elimination vs. substitution. Typical reactions in organic synthesis.

Unit 3

Substitutions on aromatic carbon: Mechanism of electrophilic, nucleophilic and free radical substitutions – orientation and reactivity. Typical reactions in organic synthesis.

Unit 4

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, Fries, Baeyer-Villiger rearrangements. Fritsch-Buttenberg-Wiechell rearrangement, Corey-Fuchs reaction, Seyferth-Gilbert homologation, Grubbs catalysts and olefin metathesis.

Unit 5

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. J. March Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 7th ed. Wiley, 2013.
2. T. H.Lowry, K.S.Richardson, Mechanism and Theory in Organic Chemistry, 3rd ed., Benjamin-Cummings Publishing Company,1997.
3. F. A. Carey, R. J. Sundberg, Advanced Organic Chemistry (parts A and B), 5th ed., Springer, 2008.
4. E. V. Anslyn, D. A. Dougherty, Modern Physical Organic Chemistry. University Science Books, 2006.
5. F. A. Carroll, Perspectives on structure and mechanism in organic chemistry, Wiley, 2011.
6. N. S. Issacs, Physical Organic Chemistry, 2nd ed., Prentice Hall, 1995.
7. A. Pross: Theoretical and Physical Principles of Organic Chemistry, 1st ed., Wiley, 1995.
8. J. Clayden, N. Green, S. Warren, P. Wothers, Organic Chemistry, 2nd ed., Oxford University Press, 2012.
9. I. Flemming, Frontier orbitals and organic chemical reactions, Wiley-Blackwell, 1976.
10. I. Flemming: Molecular orbitals and organic chemical reactions, student ed., Wiley, 2009.
11. J. McMurry, Organic Chemistry, 5th ed., Brooks/Cole, 2000.
12. R. Bruckner, Advanced organic chemistry: Reaction Mechanisms. Academic Press, 2001.
13. P. Sykes, Guidebook to Mechanism in Organic Chemistry, 6th ed., Prentice Hall, 1986.
14. N. J. Turro, Modern Molecular Photochemistry, University Science Books, 1996.
15. N. J. Turro, J.C. Scaiano, V. Ramamurthy, Modern Molecular Photochemistry of Organic Molecules, 1st ed., University Science Books, 2010.

CORE

CHE 2204 Organic Chemistry-III

(Reagents and Synthesis)

(2 Credit) **32 Hours**

Unit 1

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.

Unit 2

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 3

Chemistry of carbonyl compounds: Reactivity of carbonyl groups in aldehydes, ketones, carboxylic acids, esters, acyl halides, amides. Substitution at carbonyl carbon, mechanisms of ester hydrolysis, Substitution at α-carbon, aldol and related reactions, Stereoselective Nucleophilic Additions to Acyclic Carbonyl Croups. Cram's Rule. Felkin-Ahn Model. Effect of Chelation on Selectivity. Claisen, Darzen, Dieckmann, Perkin, Prins, Mannich, Stork-enamine reactions. Conjugate additions, Michael additions and Robinson annulation. Reaction with phosphorous and sulfurylides.

Unit 4

Protecting groups, functional group equivalents, reversal of reactivity (Umpolung), Chemistry of Nucleophilic Heterocyclic Carbenes (NHCs).

Introduction to Asymmetric Synthesis, Stereospecific and Stereoselective Synthesis, Principles, General strategies: Chiral Pool strategy, Chiral Auxiliaries, Chiral Reagents and Chiral catalysts.

Unit 5

Synthetic strategies: Introduction to retrosynthesis, strategic bond analysis, synthesis of longifolene, Corey lactone, Djerassi Prelog lactone.

References:

1. M. B. Smith, Organic Synthesis, 2nd ed., McGraw-Hill, 2000.
2. T.W.Greene, PG M Wuts, Protecting Groups in Organic Synthesis, 2nd ed., John Wiley, 1991.
3. J. March, Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 7th ed. Wiley, 2013.
4. T. H.Lowry, K.S.Richardson, Mechanism and Theory in Organic Chemistry, 3rd ed., Benjamin-Cummings Publishing Company,1997.
5. F. A. Carey, R. J. Sundberg, Advanced Organic Chemistry (parts A and B), 5th ed., Springer, 2008.
6. A. Pross, Theoretical and Physical Principles of Organic Chemistry, 1st ed., Wiley, 1995.
7. T.W. G. Solomons, Fundamentals of Organic Chemistry, 5th ed., John Wiley, 1996.
8. S. Warren, Organic Synthesis: The Disconnection Approach, 2nd ed., John Wiley, 2008
9. H. O. House, Modern Synthetic Reactions, W. A. Benjamin Inc., 1972.
10. W.Carruthers, Some Modern Methods of Organic Synthesis, 4th ed., Cambridge University Press, 2004.
11. I. L. Finar, Organic Chemistry, Volumes 1 & 2, 6th ed., Pearson Education Asia, 2004.
12. I. Flemming, Frontier orbitals and organic chemical reactions, Wiley-Blackwell, 1976.
13. I. Flemming: Molecular orbitals and organic chemical reactions, student ed., Wiley, 2009.
14. J. Clayden, N. Green, S. Warren, P. Wothers, Organic Chemistry, 2nd ed., Oxford University Press, 2012.
15. P.S.Kalsi, Stereochemistry, Conformation and Mechanism, 3rd ed., New Age Publications.
16. E. L. Eliel, S. H. Wilen, Stereochemistry in Organic Compounds, John Wiley, 1994.
17. D. Nasipuri, Stereochemistry of Organic Compounds: Principles and Applications, 2nd ed., Wiley Eastern Limited, New Delhi, 1994.

CORE

CHE 2205 Physical Chemistry-II

(Statistical Thermodynamics and Electrochemistry)

(3 Credit) **48 Hours**

Unit 1

Kinetic Theory of gases, Types of molecular velocities- Most Probable Velocity, Mean velocity, r.m.s velocity, Distribution of molecular velocities and kinetic energy- Maxwell Boltzmann distribution. Effect of temperature on distribution. Calculation of most probable, average and r.m.s velocity.

Introduction to statistical Thermodynamics, Microstates and Macrostates, Probability, Thermodynamic Probability, Relation between entropy and thermodynamic probability, Statistical Interpretation of the third law of thermodynamics, Residual entropy

Unit 2

Types of statistics- Maxwell Boltzmann, Bose Einstein and Fermi Dirac Statistics, Comparison of statistics. Dilute system concept.

Partition Function, Molecular partition function. Translational, Rotational and Vibrational Partition Function, Relation between partition function and thermodynamic properties, Localised and Delocalised systems- partition function. Partition function and equilibrium constant.

Unit 3

Heat capacity of gases- anomalous heat capacity of H_2. Heat Capacity of solids- Dulong-Petit's Law, Einstein's Theory and Debye Theory.

Applications of B.E and F.D Statistics - Bose-Einstein Condensation, Electron gas concept- Contribution to pressure and heat capacity.

Partition function for dependent particles- configurational partition function and configurational integral, communal entropy (basic concept)

Unit 4

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 behaviour, Relaxation and electrophoretic effect, Debye-Huckel-Onsager equation and its derivation. Debye Falkenhagen effect. Wein effect.

Unit 5

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. Overpotential 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 metal halide cell. Fuel Cell. Theory and working of fuel cell. H_2- O_2 fuel cell, methanol fuel cell, Solid oxide fuel cells.

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. M. Dole, Introduction to Statistical Thermodynamics, Prentice Hall, London, 1997.
4. L.K. Nash, Statistical Thermodynamics, Addison Wesley, New York, 1999.
5. J. Kestin, J.R. Dorfman, A Course in Statistical Thermodynamics, Academic press, 1971.
6. D. A. McQuarrie, Statistical Mechanics, Harper and Row, New York, 1976.
7. J. Bockris, A.K.N. Reddy, Modern Electrochemistry, 2nd ed., Wiley, New York, 1998.
8. R Crow, Principles and Applications of Electrochemistry, 4th ed., 1994.
9. S.Glasstone, An Introduction to Electrochemistry, Paperback ed., 2007.

CORE

CHE 2206 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 λ_{max} of substituted aromatic ketones, aldehydes and acids. Fluorescence Spectroscopy.

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

Unit 2

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.
IR spectra of chemical classes including amino acids.

Unit 3

Magnetic nuclei with special reference to ^{1}H and ^{13}C nuclei. Chemical shift and shielding/deshielding, relaxation processes, chemical and magnetic non-equivalence, local diamagnetic shielding and magnetic anisotropy. Proton and ^{13}C NMR scales, characteristics of ^{13}C as a nucleus.

Spin-spin splitting, AX, AX_2, AX_3, A_2X_3, 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

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

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

References

1. D.L.Pavia, G.M.Lampman, G.S.Kriz, J.R. Vyvyan, Introduction to Spectroscopy: A Guide for Students of Organic Chemistry, Indian ed., Brooks/ Cole Cengage Learning, 2007.
2. Atta-Ur-Rahman, M.I.Choudhary, Solving Problems with NMR Specroscopy, Academic Press, New York, 1996.
3. L D Field; S Sternhell, J R Kalman; Organic Structures from Spectra, 4th ed., Wiley 2008.
4. R. S. Drago, Physical Methods for Chemist, Saunders,1992.
5. C. N. Banwell, E. M. McCash, Fundamentals of Molecular Spectroscopy, 4th ed., McGraw-Hill, 1994.
6. D.F.Taber, Organic Spectroscopic Structure Determination, A Problem Based Learning Approach, Oxford University Press, 2009.
7. R. M. Silverstein, G.C. Bassler, T. C. Morril, Spectroscopic Identification of Organic Compounds, John Wiley, 1991.
8. D. H. Williams, I. Fleming, Spectroscopic Methods in Organic Chemistry, Tata McGraw Hill, 1988.
9. W. Kemp, Organic Spectroscopy, 2nd ed., ELBS-Macmillan, 1987.
10. F. Bernath, Spectra of Atoms and Molecules, 2nd ed., Oxford University Press, 2005.
11. E. B. Wilson, Jr., J. C. Decius, P. C. Cross, Molecular Vibrations: The Theory of Infrared and Raman Spectra, Dover Publications, 1980.
12. A. Weil, J. R. Bolton, Electron Paramagnetic Resonance: Elementary Theory and Practical Applications, 2nd ed., Wiley Interscience, John Wiley & Sons, Inc., 2007.
13. C. P. Slichter, Principles of Magnetic Resonance, 3rd ed., Springer-Verlag, 1990.
14. H. Gunther, NMR Sprectroscopy: Basic Principles, Concepts and Applications in Chemistry, 3rd ed., Wiley- VCH, 2013.
15. Spectral data bases (RIO DB of AIST, for example)

CORE

CHE 2207 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, FTIR, FTNMR and Mass Spectrometry.

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. A.I Vogel, A.R Tatchell, B.S Furnis, A.J, Hannaford, P.W.G. Smith, Vogel's Textbook of Practical Organic Chemistry, 5th ed., John Wiley, 1989.
2. D. L. Pavia, G. M. Lampman, G. S. Kriz, Introduction to Organic laboratory Techniques, 3rd ed., Saunders Golden Sunburst Series.
3. L. W. Harwood, C. J. Moody, Experimental Organic Chemistry-Principles and Practice, Blackwell Science Publications.

ELECTIVE

CHE 2208 Introduction to Theory of Orbital Interactions in Chemistry

(2 Credit) **32 Hours**

Unit 1

Atomic and Molecular Orbitals, Concepts of Bonding and Orbital Interaction, Orbital Interaction Energy, Molecular Orbital Coefficients, Electron Density Distribution, Perturbational Molecular Orbital Theory, Linear H_3, HF, and the Three-Orbital Problem.

Unit 2

Molecular Orbital Construction from Fragment Orbitals, Triangular H_3, Rectangular and Square Planar H_4, Tetrahedral and Linear H_4, Pentagonal H_5 and Hexagonal H_6, Molecular Orbitals of Diatomic Molecules and Electronegativity Perturbation, Geometrical Perturbation of Molecular orbitals, Molecular Orbitals of AH_2, Walsh Diagrams, Jahn–Teller Distortions.

Unit 3

Molecular Orbitals of Small Building Blocks, AH System, AH_3 Systems, pi-Bonding Effects of Ligands, AH_4 System, Molecules with Two Heavy Atoms, A_2H_6 Systems, Orbital Interactions through Space and through Bonds.

Unit 4

Polyenes and Conjugated Systems, Acyclic Polyenes, Huckel Theory, Cyclic Systems, Conjugation in Three Dimensions, Solids, Energy Bands, Hypervalent Molecules.

Unit 5

Transition Metal Complexes. Octahedral ML_6, pi-Effects in an Octahedron, Distortions from an Octahedral Geometry, Square Planar, Tetrahedral ML_4 Complexes, Five Coordination, Square Pyramidal ML_5 Fragment, ML_3 Fragment, ML_2 and ML_4 Fragments, M_2L_8 Dimers, CpM and Cp_2M, Isolobal Analogy.

References:

1. T. A. Albright, J. K. Burdett, M.-H. Whangbo, Orbital Interactions in Chemistry, 2nd ed., John Wiley and Sons, Inc., Hoboken, New Jersey, 2013.
2. I. Flemming, Molecular Orbitals and Organic Chemical Reactions, Students ed., Wiley, 2009.
3. A. Rauk, Orbital Interaction Theory of Organic Chemistry, 2nd ed., Wiley-Blackwell, 2000.
4. W. L. Jorgensen, L. Salem, The Organic Chemist's Book of Orbitals, Academic Press, 1973.

ELECTIVE

CHE 2209 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.

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 3

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 4

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 5

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 ed. 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 ed., Wiley, New York, 1992.
5. J. M. J. Cowie, Polymers. Physics and Chemistry of Modern Materials, 3rd ed., CRC Press, Boca Raton, 2007.
6. S. O. Kasap, Principles of Electronic Materials and Devises, Mc Graw Hill, 2006.

ELECTIVE

CHE 2210 Stereoselective Synthesis

(2 Credit) **32 Hours**

Unit 1

Reaction Mechanisms and Conformational Effects on Reactivity - Ester Hydrolysis, Alcohol Oxidations, S_N2 Reactions, Elimination Reactions, Epoxidation by Intramolecular Closure of Halohydrins, Epoxide Openings (S_N2), Electrophilic Additions to Olefins, Rearrangement Reactions, Conformational and Stereoelectronic Effects on Reactivity.

Unit 2

Pericyclic Reactions. Stereochemistry of Diels-Alder Reaction. Substituent Effect on Reactivity, Regioselectivity and Stereochemistry. Orbital Symmetry Basis for the Stereospecificity of Electrocyclic Reactions. Orbital Description of Sigmatropic Rearrangements. Orbital Correlation Diagram.

Unit 3

Enantiomers and Diastereomers. Resolution Methods. Stereospecific and Stereoselective Synthesis, Introduction to Asymmetric Synthesis, Principles, General strategies, Chiral Pool strategy, Chiral Auxiliaries-Diels Alder Reaction, Chiral Reagents – Binol Derivatives of $LiAlH_4$, Chiral Catalysts – CBS Catalyst.

Unit 4

Stereoselective Nucleophilic Additions to Acyclic Carbonyl Croups. Cram’s Rule. Felkin-Ahn Model. Effect of Chelation on Selectivity. Diastereoselectivity in Aldol Reactions. Stereoselective Reactions of Acyclic Alkenes. The Houk Model.

Unit 5

Stereoselective Reactions of cyclic compounds. Reactions on Small Rings. Stereochemical Control in Six Membered Rings. Stereochemistry of Bicyclic Compounds. Reactions with Cyclic Intermediates/Transition states.

References:

1. J. March, Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 7^{th} ed. Wiley, 2013.
2. T. H.Lowry, K.S.Richardson, Mechanism and Theory in Organic Chemistry, 3^{rd} ed., Benjamin-Cummings Publishing Company,1997.
3. F. A. Carey, R. J. Sundberg, Advanced Organic Chemistry (parts A and B), 5^{th} ed., Springer, 2008.
4. E. V. Anslyn, D. A. Dougherty, Modern Physical Organic Chemistry. University Science Books, 2006.
5. F. A. Carroll, Perspectives on Structure and Mechanism in Organic Chemistry, Wiley, 2011.
6. N. S. Issacs, Physical Organic Chemistry, 2^{nd} ed., Prentice Hall, 1995.
7. A. Pross, Theoretical and Physical Principles of Organic Chemistry, 1^{st} ed., Wiley, 1995.
8. J. Clayden, N. Green, S. Warren, P. Wothers, Organic Chemistry, 2^{nd} ed., Oxford University Press, 2012.
9. P.S.Kalsi, Stereochemistry, Conformation and Mechanism, 3^{rd} ed., New Age Publications.
10. E. L. Eliel, S. H. Wilen, Stereochemistry in Organic Compounds, John Wiley, 1994.
11. S. H. Pine, Organic Chemistry, 5^{th} ed., McGraw Hill, 2008.
12. I. Flemming: Molecular orbitals and organic chemical reactions, student ed., Wiley, 2009.
13. J. McMurry, Organic Chemistry, 5^{th} ed., Brooks/Cole, 2000.
14. D. Nasipuri, Stereochemistry of Organic Compounds: Principles and Applications, 2^{nd} ed., Wiley Eastern Limited, New Delhi, 1994.
15. M. B. Smith, Organic Synthesis, 2^{nd} ed., McGraw-Hill, 2000.

ELECTIVE

CHE 2211 Polymer Technology

(2 Credit) **32 Hours**

Unit 1

Classification of elastomers. Manufacture, properties, processing, compounding, vulcanisation and applications of SBR, polybutadiene and polyisoprene rubber. Comparison of synthetic polyisoprene with NR. Manufacture, properties, processing, compounding, vulcanisation and applications of EVA, Polyacrylate rubbers, Polysulphide rubbers and Polyurethanes.

Unit 2

Manufacture, properties, processing, compounding, vulcanisation and applications of EPDM, Butyl rubber, Nitrile rubber, Neoprene rubber, Hypalon rubber, Silicone rubber and Fluorocarbon rubber.

Unit 3

Brief history of plastics - Advantages and disadvantages - thermoplastics and thermosets. Manufacture of monomers, polymerization and structure of poly vinyl chloride, characterization of commercial polymers, compounding ingredients, PVC formulations. Some simple moulding techniques- Injection moulding, Compression moulding, and Blow moulding.

Unit 4

Manufacture of phenolic resins, preparation of phenol formaldehyde moulding powders, applications of PF resin. Urea formaldehyde resin and applications of UF resin. Adhesives-adhesive bonding-advantages-adhesive classification - basic terminology-theories of adhesion-wettability -performance of adhesives -shear, peel and cleavage properties-factors affecting adhesive performance. Structural adhesive -types -epoxy, urethane, acrylic, phenolic and high temperature and PVC plastisol types, advantages and disadvantages.

Unit 5

Mechanical properties of plastics and rubber – tension, compression, shear, flexural, tear strength,dynamic stress- strain, hardness, impact strength, resilience, abrasion resistance, creep and stress relaxation, compression set, dynamic fatigue, ageing properties etc. Thermal properties– specific heat, thermal conductivity, thermal expansion, heat deflection temperature etc. Electrical properties– resistivity, dielectric strength, dielectric constant etc. Optical properties – transparency, refractive index, haze, gloss etc.

References

1. W. Hofman, Rubber Technology Handbook, Hanser Publications, 1989.
2. C M Blow, Rubber Technology and Manufacture, Butterworths, London, 1971.
3. J. A.Brydson, Plastics Materials, Butterworth Heinmann, 1999.
4. H. Ulrich, Industrial Polymers - Hanser Pub. Munich, N.Y, 1982.
5. G. L. Schnberger, Adhesives in manufacturing, Marcel Dekker Inc., New York, 1983.
6. W.C.Wake, Adhesion and the formulation of adhesives, Applied Science Publishers, London, 1976.
7. R.P.Brown, Plastic Test Methods, Harlond, Longman Scientific, 1992.
8. V. Shah, Handbook of Plastic Testing Technology, John Wiley & Sons, New York, 1998.
9. R.P.Brown, Physical Testing of Rubbers, Chapman Hall, London, 1996.
10. J.F.Rabek, Experimental methods in Polymer Chemistry, John Wiley & Sons, New York, 1980.
11. F.Majewska, H.Zowalletal, Handbook of Analysis of Synthetic Polymers and Plastics, Ellis Horwood Limited Publisher, England, 1977.
12. C.A. Harper, Handbook of Plastics Elastomers & Composites, 2nd ed., McGraw Hill Inc. New York 1992.
13. M. Morton, Van Nostrand Reinhold, Rubber Technology Handbook, 1987.
14. V. R. Gowariker, N. V. Viswanathan, J.Sreedhar, Polymer Science, Wiley Eastern Limited, New Delhi, 1986.

ELECTIVE

CHE 2212 Bioanalytical Chemistry

(2 Credit) **32 Hours**

Unit 1

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

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

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

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

Unit 5

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

References

1. V. A. Gault, N. H. Mcclenaghan, Understanding Bioanalytical Chemistry-Principle and Applications, John Wiley and Sons, Ltd. Publications, 2009.
2. A. Manz, Nicole Pamme. Dimitri Iossifidis, Bioanalytical Chemistry, 2004.
3. S. R. Mikkelsen, E. Corton, Bioanalytical Chemistry, 2^{nd} ed., John Wiley and Sons, Ltd Publications, 2016.
4. Keith Wilson, John Walker, Practical Biochemistry-Principles and Techniques: 5^{th} ed., Cambridge University Press, 2000.

ELECTIVE

CHE 2213 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 –

Unit 3

Photochemistry and Photophysics of Semiconductors – Semiconductor Photocatalysis and applications. Atmospheric photochemistry.

Unit 4

Photochemistry and Advanced Materials - 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.- Photoresists – Photolithography – Photochromism – Photonic Materials and Lasers

Unit 5

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

References:

1. N. J. Turro, V. Ramamurthy, J. C. Scaiano, Modern Molecular Photochemistry of Organic Molecules, University Science Books, 2010.
2. C.E. Wayne, Photochemistry (Oxford Chemistry Primers), Oxford University Press; 1st ed. 1996.
3. J. R. Lakowicz, Principles of Fluorescene Spectroscopy, Plenum Press, 3rd ed., 2010.

4. A. M. Braun, M.-T. Maurette, Esther Oliveros, Photochemical Technology, John Wiley & Sons, 1991.
5. M.A. Fox, M. Chanon, Photoinduced Electron Transfer Part A, B. C and D, Elsevier Science Publishing Company, 1988.
6. J. Mattay Ed., Photoinduced Electron Transfer 1-5 (Topics in Current Chemistry), Springer, 1st ed., 1990-1993.
7. G. J. Kavarnos, Fundamentals of Photoinduced Electron Transfer, 1st ed., Wiley-VCH, 1993.
8. V. Ramamurthy, K. Schanze, Molecular and Supramolecular Photochemistry, Volume 10, Semiconductor Photochemistry and Photophysics, Marcel Dekker, New York, 2003.
9. V. Ramamurthy, Photochemistry in Organized and Confined Media, VCH Publishers, New York, 1991.

INTERDEPARTMENTAL ELECTIVE

CHE 2214 Chemical Instrumentation

(Credit 2) **32 hours**

Unit 1

Chromatography basic principle – adsorption and partition chromatography, importance of column technology. Paper, thin layer and column chromatographic methods, Liquid chromatography, normal phase versus reversed phase chromatography. Gas chromatography, theory and equipment, different columns used in GC. Ion exchange chromatography- basic principle. Instrumentation and applications of HPLC, LC-MS, GC-MS.

Unit 2

Basic theory and instrumentation of UV-VIS, IR. Atomic spectroscopy - atomic absorption, atomic emission. Flame emission and atomic absorption spectrometry. Instrumentation for AAS. The flame characteristics. Hollow cathode lamp. Interference in AAS. Application of AAS. Comparison between AAS and AES. ICP AES – Principle and applications.

Unit 3

Use of X-ray diffraction in structure determination (both single crystal and powder methods). Use of SEM, STM, AFM and TEM for the characterization of surfaces (Basics only). Photo electron spectroscopy- XPS and UPS (principle and applications).

Unit 4

Principles of TG and DTG, DTA and DSC, Application of TG – quantitative analysis of a mixture of Ca, Sr and Ba, decomposition of CaC2O4.H2O. Application of DTA – characterization of polymers. Application of DSC – glass transition temperature, crystallinity and crystallization rate

Unit 5

Polarography – diffusion current, supporting electrolyte, three electrode system, Polarographic maxima. Amperometry – principles and applications – Types of amperometry. Cyclic voltammetry – principles, applications. Stripping voltammetry.

References

1. J. Cazes, Marcel Dekker (Eds.) Analytical Instrumentation Hand Book, 3rd ed., New York, 2004

2. H. H. Willard, L. L. Merritt, Jr., F. A. Settle, Jr., Instrumental Methods of analysis, 7th ed., CBS Publishers & Distributors, New Delhi,1998.
3. A. Braithwaite, F.J. Smith, Chromatographic Methods, 5th ed., Black academic & Professional, 1996.
4. G. D Christian, Analytical Chemistry, John Wiley & Sons, 6th ed., 2007.
5. D. P. Woodruff, T.A. Delchar, Modern Techniques of Surface Science, 2nd ed., Cambridge University Press, 1994.
6. D.A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, Fundamentals of Analytical Chemistry, 8th ed., Saunders College Pub., 2007.

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 ed., Saunders College Pub., 2007.
2. J.R.Lakowicz, Principles of Fluorescence Spectroscopy, 3rd ed., Springer 2006.
3. G.D Christian, Analytical Chemistry, 6th ed., John Wiley & Sons, 2007.
4. M. V. Cases, Principles of Analytical Chemistry, Springer, 2000.
5. J.- M. Mermet, M. Otto, R. Kellner, Analytical Chemistry, Wiley-VCH, 2004
6. H. Gunzler, A. Williams, Handbook of Analytical Techniques, Volume 2, Wiley-VCH, 2001.
7. S. Higson, Analytical chemistry, OUP Oxford, 2003.
8. A. Zschunke, (Eds), Reference Materials in Analytical Chemistry, Springer, 2000.

CORE

CHE 2302 Inorganic Chemistry- III

(Organometallic and Bioinorganic Chemistry)

(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, carbenes and 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, 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, J. S. Valentine, Bioinorganic Chemistry, Viva Books.
4. R. W. Hay, Bio Inorganic Chemistry, Ellis Horwood, 1987.
5. J.E. Huheey, E. A. Keiter, R. L. Keiter, Inorganic Chemistry: Principles of structure and Reactivity", 4th ed., Harper Collin College Publishers, 1993.
6. J. A. Cowan, Inorganic Biochemistry - An Introduction, 2nd ed., VCH, 1997.
7. N. 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 Chemistry of Life, John Wiley 1994.

CORE

CHE 2303 ORGANIC CHEMISTRY-IV

(*Natural Products*)

(4 Credit) **64 hours**

Unit 1

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

Unit 2

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

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

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

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. B. Smith, Organic Synthesis, 2nd ed., McGraw-Hill, 2000.
2. F. A. Carey, R. J. Sundberg, Advanced Organic Chemistry (parts A and B), 5th ed., Springer, 2008.
3. T.W. G. Solomons, Fundamentals of Organic Chemistry, 5th ed., John Wiley
4. H. O. House, Modern Synthetic Reactions, W. A. Benjamin Inc., 1972.
5. W.Carruthers, Some Modern Methods of Organic Synthesis, 4th ed., Cambridge University Press, 2004.
6. I. L. Finar, Organic Chemistry Volumes 1 & 2, 6th ed., Pearson Education Asia, 2004.
7. J. Clayden, N. Green, S. Warren, P. Wothers, Organic Chemistry, 2nd ed., Oxford University Press, 2012.
8. N. R. Krishnaswamy, Chemistry of Natural Products; A Unified Approach, Universities Press, 1999.
9. R. J. Simmonds, Chemistry of Biomolecules: An Introduction, RSC, 1992.
10. R. O. C. Norman, Principles of Organic Synthesis, 2nd ed., Chapman and Hall, 1978.
11. J. A. Joule, K. Mills, Heterocyclic Chemistry, 5th ed., Wiley, 1998.

CORE

CHE 2304 Physical Chemistry-III

(Kinetics, Surface Chemistry and Catalysis)

(3 Credit) **48 Hours**

Unit 1

Complex reactions- Steady State Approximation, Concurrent, Consecutive and Reversible reactions. Theories of unimolecular reaction and termolecular reaction.

Kinetics of Chain Reactions- Thermal and Photochemical reactions- H_2-Cl_2 and H_2-Br_2, Quantum yield, Organic Decomposition Reactions- Rice Herzfeld Mechanism. Branching Chain Reactions- H_2-O_2 reaction.

Fluorescence and Phosphorescence- Quenching, Stern Volmer equation. Delayed Fluorescence-N and P type.

Fast reactions and relaxation methods.

Unit 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.

Unit 3

Reactions in solution- Cage effect, Transition state theory for reactions in solution. Influence of solvents, Diffusion controlled reactions, Effect ionic strength, dielectric constant and internal pressure- Primary salt effect.

Unit 4

s

Different types of interfaces, Surface tension, Surface films, Surface potential, Surface excess. Adsorption- Physisorption and chemisorption, Adsorption Isotherms – Langmuir (kinetic and statistical derivation), Freundlich and BET isotherms (derivation). Determination of surface area from isotherms, Isosteric heat of adsorption, Gibbs adsorption isotherm.

Unit 5

Catalysis – Homogeneous and heterogeneous. Homogeneous catalysis- acid base and enzyme catalysis. Secondary Salt effect, Heterogeneous Catalysis- Mechanism of heterogeneous catalysis. Eley-Rideal and Hinshelwood mechanisms. Inhibition- Competitive and noncompetitive, Autocatalysis – Oscillatory reactions- Lotka-Volterra, Oregonator, Brussellator.

References:

1. W. J. Moore, R. G. Pearson, Kinetics and Mechanism, Wiley, New York, 1988
2. K. J. Laidler, Chemical Kinetics, McGraw Hill, New York, 1991.
3. F. Daniels, R. A. Alberty, Physical Chemistry, 8^{th} ed., Wiley, New York, 1994.
4. P. W. Atkins, Physical Chemistry 8^{th} ed., Wiley, New York, 2006
5. A. W. Adamson, The Physical Chemistry of Surfaces, 2^{nd} ed., Wiley. New York, 1998.
6. A. Somorjai, Chemistry of Surfaces, 3^{rd} ed., Wiley, New York, 2005.
7. A. Alexander, P. Johnson, Colloid Science, Oxford University Press, Oxford, New York, 1996.

CORE

CHE 2305 Physical Chemistry Lab

(2 Credit)

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.

   Hydrolysis of p-nitrophenyl acetate using spectrophotometry

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

7. Conductometry : Cell constant, conductivity of a weak-acid, solubility of a sparingly soluble salt, conductometric titrations. Determination of critical miscelle concentration of colloids.

8. Poteniometry : Measurement of electrode potentials, activity coefficients and potentiometric titrations, pH metric titrations.

9. Spectrophotometry

10. Flame photometry

11. AAS

References:

1. A.Findlay, Practical Physical Chemistry, Longman.
2. F.Daniels et al Experimental Physical Chemistry, McGraw Hill.
3. D. P. Shoemaker, C.W. Garland, J.W, Nibler, Experiments in Physical Chemistry, 5th ed., McGraw Hill, 1989.
4. J B Yadav, Advanced Practical Physical Chemistry, Paperback ed., 2016.
5. J. N. Gurtu, A.N. Gurtu, Advanced Physical Chemistry Experiments, Pragati Prakashan, 2011.

ELECTIVE

CHE 2306 Nuclear and Radiation Chemistry

(3 Credit) **48 Hours**

Unit 1

Elementary particles, Nuclear Stability- N/P ratio, Even Odd nature, Nuclear potential, Binding energy, Separation energy systematics, abundance systematics, exchange theory, Nuclear models-liquid drop model, shell model, semi-empirical mass equation, Nuclear properties- nuclear radius, mass, dipole moment, nuclear spin, magnetic moment, quadrupole moment and shape of nucleus.

Unit 2

Radioactivity – Types of decay, decay kinetics, kinetics of mixture of unrelated nuclides, parent daughter decay growth relationship, reaction cross section-compound nucleus theory, high energy nuclear, direct nuclear, photonuclear and thermonuclear reactions. Artificial transmutation and artificial radioactivity.

Unit 3

Types of nuclear reactions: 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 fuel, neutron source, chemistry of operating reactor, nuclear power plant - nuclear reactors in India. Fusion reactions, hydrogen bomb and energy of sun, radioactive waste disposal.

Unit 4

Detection and measurement of activity- Scintillation, semiconductor, thermoluminesence and neutron detector, Isotopes for reactors, preparation of radioisotopes, isotope separation, Transuranium elements, Limits of Stability, Element synthesis, super heavy elements

Unit 5

Radiation chemistry- interaction of radiation with matter, radiation dosimetry, radiolysis of water, radiation induced damage. Applications of Radioactivity – Carbon dating, rock dating, NAA, Radiopharmaceuticals, RIA, Nuclear Forensics, surface area and solubility determination.

References

1. H. J. Arnikar, Essentials of Nuclear Chemistry, 4th ed., New Age International, 2011.
2. W. D. Loveland, D. J. Morrissey, G. T. Seaborg, Modern Nuclear Chemistry, 2nd ed., Wiley, 2017.
3. K. H. Lieser, Nuclear and Radiochemistry, 2nd ed., Wiley VCH, 2001.
4. D. I. Coomber, Radiochemical Methods in Analysis, PLENUM PRESS, 1975.
5. J. F. Wishart, B. S. M. Rao, Recent Trends in Radiation Chemistry, World Scientific, 2011.

ELECTIVE

CHE 2307 Industrial Catalysis

(3 Credit) **48 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

Catalyst preparation methods – precipitation and coprecipitation – mechanism of nuclear formation and crystal growth, Sol gel process, Hydrothermal/ solvothermal process.

Dispersed metal catalysts; Support materials; preparation and structure of supports; Synthesis of aluminosilicate zeolites and related silica-based materials, Mesoporous materials - synthesis of silica and carbon molecular sieve materials. Characterization of mesoporous molecular sieves. Carbon based nanomaterials- CNT, graphene, Quantum dots.

Unit 3

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.

Enzyme catalysis: Introduction to enzymes as proteins, 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 – enzyme kinetics as an approach to understanding mechanism. Characteristics of immobilized biocatalysts – activity and stability as a function of temperature

Principles of photochemistry- Franck Condon principle, Jablonski diagram, Beer Lambert Law, Quantum yield, Quenching and sensitization, Stern Volmer plots, Photoinduced electron transfer reactions, Photoelectrochemical Properties, Semiconductor photocatalysis. Photocatalysis for environmental remediation/ energy applications.

Unit 4

General Principles and Application in catalysis - XRD, FTIR, Electronic spectroscopy, SEM, TEM, XPS, Thermogravimetric studies, Thermal desorption for surface characterization.

Unit 5

Industrially important processes- Catalytic cracking, Catalytic reforming, Isomerisation, Hydrodesulphurisation, Mobil process for conversion of methanol to gasoline.

Deactivation of catalysts, classification of catalyst deactivation processes, poisoning, coke formation, metal deposition, sintering, Regeneration of deactivated catalysts.

References

1. R. Pearce and W.R. Patterson, Catalysis and Chemical Processes, Academic press, Leonard Hill, London, 1981.
2. A. Clark, Theory of Adsorption and Catalysis, Academic Press, New York, 1970.
3. J.M. Thomas, W.J. Thomas, Introduction to Principles of Heterogeneous Catalysis, Academic Press, New York, 1967.
4. D.K Chakraborthy, Adsorption and Catalysis by Solids, Wiley Eastern Ltd. 1990.
5. J.R. Anderson, M. Boudart (Eds), Catalysis: Science and Technology, Vol 6, Springer-Verlag, Ber lin Heildberg, 1984.
6. R. Szostak, Molecular Sieves: Principles of Synthesis and Identification, Van Nostrand, NY, 1989.
7. R. Hughes, Deactivation of catalysts, Academic press, London, 1984.
8. A.L. Lehninger, Principles of Biochemistry, Worth Publishers, USA, 1987.
9. C.M. Starks, C.L. Liotta, M. Halpern, Phase Transfer Catalysis – Fundamentals, applications and Industrial Perspectives, Chapman & Hall, New York, 1994.
10. N. J. Turro, V. Ramamurthy, J. C. Scaiano, Modern Molecular Photochemistry of Organic Molecules, University Science Books, 2010.
11. M. Kaneko, I. Okura, Photocatalysis: Science & Technology, Springer, 2002.
12. M. Schiavello, Heterogeneous Photocatalysis, Wiley, 1995.
13. D.P. Woodruff, T.A. Delchar, Modern Techniques of Surface Science, Cambridge, University Press, 1990.
14. J.W. Niemantsverdriet, Spectroscopy in Catalysis: an Introduction, VCH, NY, 1995.
15. G. Ertl, H. Knozinger and J. Weitkamp, Handbook of Heterogeneous Catalysis, Vol 2 & 3, Wiley-VCH, Weinheim, 1997.

ELECTIVE

CHE 2308 Medicinal Chemistry

(4 Credit) **64 Hours**

Unit I

Principles of Drug discovery: Introduction to drug discovery. drug discovery without lead – serendipity – Pencillins, Cisplatin, librium (chlordiazepoxide), aspertame as examples. Selection of disease and drug target. Bioassay and Lead discovery. Drugs from natural sources and development. Bioinformatics- introduction, Molecular basis of disease, Molecular basis of curing disease, developing drugs.

Case studies of modification of morphine and atropine. Drug metabolism studies: Phase I and Phase II metabolism. Clinical observations: Phase I, Phase II, Phase III, Phase IV trials. Principles of drug design; agonist, antagonist drugs, Structure pruning technique in drug design (eg. morphine pharmacophore). Development of ranitidine and captopril from lead molecules. Introduction to combinatorial synthesis. Drug resistance and mutation.

Unit 2

Introduction to structure-activity relationship (SAR) studies – (i) Binding role of hydroxyl group, amino group, aromatic ring, double bond, ketones and amides, (ii) Variation of substituents – alkyl substituents, aromatic substituents, extension of structure, chain extension / contraction, ring expansion / contraction, ring variation, ring fusion, Isosteres. (iii) Simplification of the structure, rigidification, conformational blockers. X-ray crystallographic studies. Case studies of oxaminquine (schistosomiasis), sulpha drugs (antibacterial), benzodiazepines (hypnotic).

Unit 3

Introduction to Quantitative Structure Activity Relationship (QSAR) studies. QSAR parameters – substituent constants – linear and non – linear relationships between ρ and biological activity. Electronic parameters, steric parameters, effect of electronic and steric parameters on lipophilicity. Methods used in QSAR studies – (i) Linear free energy relationship (LFER). Application of Hammett equation. (i) Hansch analysis – significance of slopes and intercepts in Hansch analysis, (ii) Craig's plot, (iii) Topliss scheme, (iv) Free Wilson model – advantages and disadvantages, (v) Clustet significant analysis (vi) Minimal topological difference method.

Unit 4

Chemotherapeutic Agents – Synthetic DNA targeted agents, Radiosenzitizers and Radioprotective agents, Antitumor natural products, HIV Drugs, β-lactum antibiotics, Selective toxicity, Organ transplant drugs, Antifungal, Antiprotozoal, Antimalarial, Antimycobacterial, Anthelmintics**.**

Introduction to chiral drugs. Eotomer, distomer, eudesmic ratio, three point contact model – Feiffers rule. **[Introductory with two examples]**

Unit 5

Penicillins, cephalosporins, valinomycin, gramicidin, tetracyclins, chloramphenicol, erythromycin, ciprofloxacin, isoniazid, prontosil (Antibacterial agents). Ivermectin (antiparasitic) Aspirin (analgesic), Aciclovir, azidothymidine, saquinavir, ritonavir, oseltamivir (Antiviral agents).Genistein, camptothecin, podophyllotoxin, calicheamicin, tamoxifen, paclitaxel (Anticancer agents). Salbutamol, ephedrine, Phenobarbital, prozac (CNS Drugs).Salvarsan (Antisyphilitic). Lovastatin (cholesterol lowering), cyclosporine (immunosuppressant).Viagra (vascodialator).Methadone (narcotic). **[ANY FIVE]**

References:

1. G. L. Patrick, An Introduction of Medicinal Chemistry, 3rd ed., Oxford International Edition, Oxford University Press, 2006.
2. T. Lengauer, R. Mannhold, H. Kubinyi, H.Timmerman, Bioinformatics – From Genes to Drugs, Wiley VCH, 2002.
3. R. B. Silverman, Organic Chemistry of Drug Design and Action, 2nd ed., Academic Press, Sandiego, 2004.
4. D. J. Abraham, Burger's Medicinal Chemistry and Drug Discovery, Chemotherapeutic Agents, Wiley-Interscience, 2003.
5. G. Thomas, Medicinal Chemistry: An Introduction, 2nd ed., John Wiley and Sons, 2007,
6. D. J. Abraham, Berger’s Medicinal Chemistry, 6th ed., Vol 1-6, John Wiley and Sons, New York, 2003.

ELECTIVE

CHE 2309 Solid State Chemistry and Crystallography

(4 Credit) **64 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 image formation, 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.

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

Unit 4

Crystals- Preparation 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; Microwave Irradiation method, Sonochemical method, preparation of thin films - electrochemical methods, chemical vapour deposition; Crystal growth - Bridgman & Stokbarger methods, zone melting.

Unit 5

Identification of crystal systems, cell parameters, asymmetric unit, unit cell, faces of crystal, Miller indices, Crystal symmetry, Space groups (symmorphic and non-symmorphic systems), reciprocal lattice, Properties of a crystal.

Significance of crystal structure determination by using X–rays as source, X-ray diffraction method- Experimental set up, Bragg's law.

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. L. Smart, E. Moore, Solid State Chemistry, Chapman and Hall, 1995.
7. H. V. Keer, Principles of the Solid State, Wiley Eastern Ltd, New Delhi, 1993.
8. R.S. Drago, Physical Methods for Chemists, 2nd ed., Sauders College Publishing, 1992.
9. A Primer, J.P. Glusker, K.N. Trueblood, Crystal Structure Analysis, 3rd ed., Oxford University Press Inc., New York, 2010.
10. C Giacavazzo, H.L. Monaco, G. Artioli, D. Viterbo, M. Milanesio, G. Ferraris, G. Gilli, P. Gilli, G. Zanotti, M. Catti, Fundamentals of Crystallography, 3rd ed., Oxford Science Publications, Oxford University Press, 2011**.**
11. J. D. Dunitz, X-ray Analysis and the Structure of Organic Molecules, 2nd ed., Wiley-VCH, 1996**.**
12. G.H. Stout, L.H. Jensen, X-ray structure determination: A Practical guide, 2nd ed., Wiley Interscience Publications, 1989**.**

ELECTIVE

CHE 2310 Molecular Modeling in Chemistry

(4 Credit) **64 Hours**

Unit 1

The Schrödinger Equation, The Time-Independent Schrödinger Equation, Born-Oppenheimer approximation, The Molecular Potential Energy Surface, Multiple Minima, Saddle Points, Characterization, Finding Minima, LCAO, Hartree-Fock theory, Roothan–Hall equations, Koopmans theorem, HF limit and electron correlation.

Unit 2

Basis sets, basis set approximation, Slater and Gaussian functions, contractions, polarization and diffuse functions, split-valence sets, classification of basis sets – minimal, double zeta, triple zeta, correlation-consistent sets, core-valence sets, general contractions, EMSL basis set exchange.

Unit 3

Semi empirical methods, post Hartree-Fock Method, Configuration interaction, Many-body perturbation theory, Coupled-cluster theory, Nondynamical correlation and multiconfigurational self-consistent-field (MCSCF) theory, Density Functional Theory, Hybrid QM/MM.

Unit 4

Input of molecular structure, Z-matrix construction, single point energy calculations, geometry optimizations, Electronic Energy, Vibrational frequency analysis, symmetry analysis, zero-point vibrational energies (ZPVE's), distinguishing minima from transition states, Intrinsic reaction coordinate (IRC) analysis, transition barrier and activation energy, conformational energetics, reaction energetics, enthalpy of formation, bond dissociation energy, ionization energy, isomerization energy and barrier, potential energy surface, reaction mechanism, enthalpy, entropy and free energy changes for reactions, isodesmic reactions.

Unit 5

Introduction to molecular mechanics; The Force Field Energy, The stretch energy, The bending energy, The out-of-plane bending energy, The torsional energy, The van der Waals energy, The electrostatic energy: charges and dipoles, Force Field Parameterization, Universal force fields, Advantages and Limitations of Force Field Methods, Basics of Molecular Dynamics Simulation, Generating and Analyzing a Molecular Dynamics Trajectory, Methods for Calculation of Free Energy, Application to Intermolecular Interactions & Binding Energies, Solvation Models, Combined QM/MM methods, Application of QM/MM to Enzyme.

References:

1. C. J. Cramer, Essentials of Computational Chemistry: Theories and Models, 2nd ed., John Wiley & Sons, 2004.
2. F. Jensen, Introduction to Computational Chemistry, 3rd ed., Wiley, New York, 2017.
3. A. R. Leach, Molecular Modelling Principles and Applications, 2nd ed., Pearson Education Limited, 2001
4. I. N. Levine, Quantum Chemistry, 7th ed., Pearson, 2013.

ELECTIVE

CHE 2311 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, S J Hall, Principle of Fermentation Technology, Elsevier, 2003.
2. J.Pelczar Jr., Reid, E.C.S.Chan, Microbiology. McGraw Hills Inc., New York, 1979.
3. L.E, Casida Industrial Microbiology, 1984.
4. H. J.Peppler, D. Perlman, Microbial Technology, Academic press, 1979.
5. J. B'uock and B. Kristansen, Basic Biotechnology, Academic Press, 1987.

ELECTIVE

CHE 2312 Chemistry of Carbohydrates

(2 Credit) **32 Hours**

Unit I

Definition and classification of sugars, nomenclature, aldoses and ketoses, configuation of (+)- glucose: the Fischer proof, ring structures and conformation, mutarotation, anomericity, naturally occurring monosaccharides, oligosaccharides and polysaccharides, three-dimensional structure of macromolecular carbohydrates. Introduction to Inositol and its derivatives and their commercial applications.

Unit 2

Methods for isolation, purification and structural analysis, complete and partial hydrolysis, methylation analysis, Smith degradation, color tests and methods for estimation of carbohydrates.

Unit 3

Chemical ractions of carbohydrates, oxidation, reduction, formation of derivatives, glycosides, ethers, esters and cyclic acetals, modern chemical transformations, methods for the formation and cleavage of O-glycosidic bond, use of protecting groups, Formation of acetals between diols, Regioselective opening and deprotection of acetals, Esterifications, Ester deprotections, Alkylations, Silylations, Nitrogen protections. Conversion of glucose to ascorbic acid.

Unit 4

Chemical and enzymatic synthesis of oligosaccharides, carbohydrates as chiral synthons for natural products synthesis.Nucleophilic Displacement on Carbohydrate Rings.

Unit 5

Carbohydrate biopolymers, animal glycoproteins, blood-group substances, plant and algal glycoproteins, proteoglycans and glycosaminoglycans, glycolipids, glycoconjugates, carbohydrate componets of nucleic acids and antibiotics.

References:

1. J.F. Kennedy, C.A. White, Bioactive Carbohydrates, Ellis Horwood, New York, 1983.
2. R.W. Binkley, Modern Carbohydrate Chemistry, Marcell and Dekker, New York,1988.

3. J.F. Kennedy (Ed.) Carbohydrate Chemistry, Oxford University Press, Oxford, 1988.

4. E.A. Davidson, Carbohydrate Chemistry, Holt, Rinehart & Winston Inc., New York, 1967.
5. A.F.Bochkov, G.E. Zaikov, Chemistry of the O-Glycosidic Bond Formation and Cleavage, Pergamon, Oxford, 1979.
6. S.Hanessian, Total Synthesis of Natural Products: The Chiron Approach, Pergamon, Oxford. 1983.
7. K, Thisbe, Essentials of Carbohydrate Chemistry and Biochemistry, 3rd ed., Lindhorst Wiley VCH 2007.
8. B. G. Davis, A. J. Fairbanks, Carbohydrate Chemistry, Oxford Chemistry Primers, Oxford University Press 2002.

SEMESTER 4

CHE 2401 Project Dissertation (16 Credit)