SAKTHI COLLEGE OF ARTS AND SCIENCE FOR WOMEN, ODDANCHATRAM

(Recognized Under Section 2(f) and 12(B) of UGC Act 1956)

(Affiliated to Mother Teresa Women's University, Kodaikanal)

PG AND RESEARCH DEPARTMENT OF CHEMISTRY

CURRICULUM FRAMEWORK AND SYLLABUS FOR

OUTCOME BASED EDUCATION IN

SYLLABUS FOR

M.Sc., CHEMISTRY

FRAMED BY

MOTHER TERESA WOMEN'S UNIVERSITY, KODAIKANAL

UNDER

CHOICE BASED CREDIT SYSTEM

2015 - 2018

Paper No.	Paper Code	Course Title	Credits	Continuous internal Assessment (CIS)	End Semester Exam (ESE)	Total
SEMESTER - I						
1	CHE011C	Organic Chemistry I	5	40	60	100
2	CHE012C	Inorganic Chemistry I	5	40	60	100
3	CHE013C	Physical Chemistry I	5	40	60	100
4	CHE014C	Organic Chemistry Practical	5	40	60	100
5	CHE015E	Medicinal Chemistry and Drug Design	5	40	60	100
		Total	**25**			
SEMESTER –II						
6	CHE021C	Organic Chemistry II	5	40	60	100
7	CHE022C	Inorganic Chemistry II	5	40	60	100
	CHE023C	Physical Chemistry II	5	40	60	100
8	CHE024C	Inorganic Chemistry Practical	5	40	60	100
9	CHE025E	Analytical Techniques	5	40	60	100
		Total	**25**			
SEMESTER – III						
11	CHE031C	Organic Chemistry III	5	40	60	100
12	CHE032C	Inorganic Chemistry III	5	40	60	100
13	CHE033C	Physical Chemistry III	5	40	60	100
14	CHE034C	Physical Chemistry Practical	5	40	60	100
15	CHE035E	Environmental Chemistry, Green Chemistry and Asymmetric synthesis	5	40	60	100

			25			
SEMESTER – IV						
16	CHE041C	Chemistry of Natural Products and Bio-inorganic chemistry	5	40	60	100
17	CHE042C	Nano chemistry & Supramolecular Chemistry	5	40	60	100
19	CHE043C	Project Work	5	40	60	100
		Total	**15**			
90						

SEMESTER – I

CHE 011C ORGANIC CHEMISTRY - I

Unit I / Reactive intermediate

Generation, stability and reactivity of carbocations, carbanions, carbenes, benzynes and nitrenes. Correlation on reactivity with structure of reactive intermediates - Free radicals – configurations – identification by chemical and spectral methods – free radical halogenations – NCS and NBS

Unit II / Aromaticity

Aromatic character: Six-, five-, seven-, and eight- membered rings - Other systems with aromatic sextets – Huckel's theory of aromaticity, concept of homoaromaticity and antiaromaticity, Electron occupancy in MO's and aromaticity - NMR concept of aromaticity and antiaromaticity, systems with 2,4,8 and 10 electrons, systems with more than 10 electrons, alternant and non-alternant hydrocarbons (azulene type). Bonding properties of systems with (4n+2)□□electrons and 4n□□electrons, Heteraromatic molecules. Annulenes, heteroannulenes, sydnones and fullerenes. Craig's rule, Hammond's postulate

Unit III / Substitution reactions

Nucleophilic Substitution

1. Aliphatic nucleophilic substitution: S_N1 and S_N2 mechanism – Kinetic and stereochemical characteristics – effects of substrate structure, nature of the nucleophile and leaving group on the rate – solvent effects – examples of S_Ni substitution – Neighbouring group participation-Anchimeric assistance
2. Aromatic nucleophilic substitution: Benzyne and Meisenheimer intermediates

Electrophilic Substitution

1. Mechanism of aliphatic electrophilic substitution reaction – S_E1, S_E2, S_Ei reaction.

Mechanism of aromatic electrophilic substitution reactions – complexes – nitration, halogenation, sulphonation, Friedel Craft alkylation and acylation – Reimer Tiemann reaction. Linear free energy relationship – Hammett equation – Significance of the σ and ρ parameters; Taft equation.

Unit IV / Addition and Elimination reactions

Addition reactions

Regio and stereochemistry of addition of halogens and halogens acids to carbon – carbon multiple bonds – hydroboration – addition to carbonyl bonds – mechanism of Aldol, Perkin, Stobbe, Dieckmann condensation, Reformatsky and Grignard reaction, Michael addition

reaction and Mannich reaction – Formation and Synthetic application of enamines – Stork enamine reaction – Mechanism of ester hydrolysis.

Elimination reactions

E1, E2, E1CB mechanism – structural and solvent effect on these mechanisms – orientation of double bonds (regio and stereoselectivities) – competition between substitution and elimination reaction – cis elimination.

Unit V / Rearrangements

Definition – nucleophilic, electrophilic and free radical rearrangements – intramolecular and intermolecular rearrangements – migratory aptitude – Wagner – Meerwin, pinacol – pinacolone, Benzil – Benzilic acid, Hofmann, Schmidt, Lossen, Curtius, Beckmann, Fries, Baeyer Villeger, Favorski, Stevens and Neber rearrangements.

Text books

1. J.March, Advanced Organic Chemistry, 4th Edn. John Wiley, New York,1992.
2. P.Sykes, A Guide book to Mechanisms in Organic Chemistry, 6th Edn., Longmans Scientific and Technical, Essex, 1986.
3. R.T.Morrison and B.N.Boyd, "Organic Chemistry", 6th Edn., Pearson,1992.

Reference Books:

1. F.S.Gould, Mechanism and Structure in Organic Chemistry, Holt, New York,1959.
2. P. Bhattacharjee, Pathway to Organic Chemistry, Strucutre and Mechanism, Books and Allied, Kolkata, India, 2012.
3. K. S. Mukerjee, Mecahnism of Organic Reactions, Books and Allied, Kolkata, India, 2010.
4. T.H.Lowry and K.S.Richardson, Mechanism and theory in Organic Chemistry, Harper and Row, New York, 1976.
5. T.W.G.Solomons, Organic Chemistry, 6th Edn., John Wiley, New York, 1996.
6. G.W.Loudon, "Organic Chemistry", 3rd edn. Benjamin-Cummings, 1995.
7. F.A.Carey and R.J.Sundberg, Advanced Organic Chemistry, Part A and Part B, 3rd Edn., Plenum press, New York, 1990.

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CHE 014C ORGANIC CHEMISTRY PRACTICALS

1. Purification techniques of organic compounds and their spectroscopic identifications.
    a) Purification of binary mixtures by Thin Layer Chromatography (TLC) and Column chromatography
    b) Purification of tertiary mixture of amino acids by paper chromatography
    (Both experiments demonstration only)
2. Extraction of natural products such as Caffeine, nicotine, piperine, carotenoids, embelin and lecanoric acid (Demonstration only)
3. Organic preparation: About 6-8 preparations (involving two or more than two steps) involving the following representative reactions-
    a) Esterification and saponification
    b) Oxidation
    c) Hydride reduction
    d) Nucleophilic substitution
    e) Cycloaddition reaction
    f) Condensation reaction
    g) Aromatic electrophilic substitution
    h) Heterocyclic synthesis
4. Qualitative analysis – Separation of two component mixture and identification of components by chemical methods (about 4 – 5 mixtures)
5. Quantitative Analysis
    a) Estimation of ketone
    b) Estimation of carboxylic acid
    c) Estimation of glucose

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INORGANIC CHEMISTRY - I

CHE012C STRUCTURE & BONDING IN INORGANIC COMPOUNDS

Unit I Covalent Bonding

V.B. approach to bonding-Hitler-London, Pauling and Slater refinements, Concept of hybridization and structure of molecules, VSEPR theory shapes of molecules. M.O. approach to covalent bonding – symmetry and overlap of atomic orbitals – symmetry of molecular orbitals – sigma and pi bonding – energy levels in homo and hetero nuclear diatomic systems – bond length, bond order and bond energy, Application to small molecules such as $BeCl_2$, BCl_3 and CCl_4, SF_4, etc, ionic character in a covalent bond - The concept of multicentre bonding.

Unit II Metallic Bonding

Drude Lorentz theorem, merits and demerits – Sommerfield theroem – band theorem – formation of Brillion Zones – conductors and insulators and semiconductors, – Hall effect – super conductors, photoconductivity. Point-, line- and plane defects in solids – Stoichiometric and non-stoichiometic defects – Frenkel and Schottky defects. Effect of imperfections on physical properties like electrical conductivity, thermal, optical and magnetic phenomena.

Unit III Solid State – Structure

Cohesive energy and Medelung constants, van der Waals forces, Close packing of atoms and ions HCP and BCC types of packing voids, radius ratio – derivation – its influence on structures. Lattice energy – Born-Lande equation - Kapustinski equation. Representative structures of AB and AB_2 types of compounds - rock salt, calcium chloride, wurtzite, zinc blende, rutile, fluorite, antifluorite, cadmium iodide and nickel arsenide. Structure of graphite and diamond. Spinels -normal and inverse types and perovskite structures.

Unit IV Main Group Chemistry

Chemistry of boron – borane, higher boranes, carboranes, borazines and boron nitrides. Chemistry of silicon – silanes, higher silanes, multiple bonded systems, silicon nitrides, siloxanes. P-N compounds, cyclophosphazenes and cyclophosphazanes. S-N compounds – S_4N_4, $(SN)_x$.

Unit V Interhalogens and Polymeric Inorganic Compounds

Pseudo halogens: Structure and bonding in ClF_3, BrF_3 , BrF_5 , IF_5, IF_7 etc . Oxides and oxoacids of halogens, Isopoly and heteropoly acids – Structure and bonding of 6- and 12 – isopoly and heteropoly anions. Structure of silicates - applications of Paulings rule of

electrovalence - isomorphous replacements in silicates – ortho, meta and pyro silicates – one dimensional, two dimensional and three dimensional silicates – Bonding in Noble gas compounds – $XeCl_2$, XeF_4, $XeOF_4$, XeF_6.,

Text Books

1. J.E. Huheey, Inorganic Chemistry, 3rd. Ed., Harper & Row publisher, 1983.
2. J.D. Lee, Concise Inorganic Chemistry, 5th Ed, Wiley, 1999.
3. William L. Jolly, Modern Inorganic Chemistry, 2nd Ed. McGraw-Hill, 1991.

Reference Books

1. D.E. Douglas, D.H. McDaniel, J.J. Alexander, Concepts and Models in Inorganic Chemistry, 3rd Ed. 1994.
2. M.C. Day, J. Selbin, Theoretical Inorganic Chemistry, 2nd Ed., East West Press, 1985.
3. F. Basolo, R.G. Pearson, Mechanism of Inorganic Reactions, 2nd Ed., John Wiley, 1967.
4. L. Pauling, The Nature of the Chemical Bond, 3rd Ed., Cornell University Press, 1960.
5. F.A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry, 4th Ed., John Wiley & Sons, 1986.
5. D.F. Shriver, P.W. Atkins, Inorganic Chemistry, 3rd Ed, 1999.
6. A.G. Sharpe, Inorganic Chemistry, Pearson Education, 2008.

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CHE013C PHYSICAL CHEMISTRY - I

Unit I Thermodynamics Chemical and Phase Equilibrium

The second law of thermodynamics – Entropy – thermodynamics of systems of variable compositions – partial molar quantities and their determination – chemical potential – Gibbs-Duhem equation – Third law of thermodynamics, exceptions and applications. Activity and Fugacity- determination of fugacity, Nernst equation, Chemical equilibrium - temperature dependence, Vant-Hoff equation, Non-equilibrium thermodynamics - postulates and methodology. Phase equilibrium-Application to three component system.

Unit II Chemical Kinetics

Derivation of rate constant for opposing, consecutive and parallel reaction - steady state approximation. Chain reactions: kinetics of decomposition of N_2O_5 – Non stationary chain reaction: H_2O_2 reaction and explosion limits. Grunwald –Winstein equation on reaction rates. Concept of Linear Free Energy Relationships - derivation of Hammett equation-significance of substituent and reaction rate constants - Taft equation - thermodynamic implications of LFER. Experimental methods for the study of fast reaction - flow method-relaxation methods.

Unit III Electrochemistry – I

Mean ion activity and activity coefficient of electrolytes in solution – Ion association - Ionic strength – Debye-Huckel theory – Debye-Huckel limiting law - its validity and limitations – Strong and weak electrolytes – Debye theory of electrolytic conductance – Debye – Huckel – Onsager equation - Verification and limitations - Electrochemical cells and applications of standard potentials. Batteries-Primary and secondary fuel cells – Corrosion and corrosion inhibition

Unit IV Electrochemistry – II

The electrical double layer – Polarizable and non-polarizable interfaces – Structure of electrical double layer – Electrocapillary and double layer capacity measurements – Double layer models – Helmholtz, Guoy–Chapman and Stern models.

Electrokinetic phenomena: Zeta potential – Electroosmosis, streaming potential, electrophoresis and sedimentation potential . Kinetics of electrode processes – Current–potential curve – Butler–Volmer relation and its approximations – Tafel equation – Charge transfer resistance – Nernst equation from Butler–Volmer equation –Multistep processes – Symmetry factor and transfer coefficient – Electrocatalysis–Hydrogen evolution reaction as a case study.

Unit V Photochemistry

Absorption of light by molecules, reaction paths of electronically excited molecules – de-excitation pathways, Fluorescence and Phosphoresence – Jablanski diagram – Physical properties of the electronic excited molecules – excited state dipole moments, excited state pKa and redox potentials – Stern – Volmer equation and its application – photosensitization – Chemi Luminescence – Quantum Yield and actinometry.

Text Books

1. P.W. Atkins,Physical Chemistry, 7th Ed., Oxford University press, 2002.
2. J. Rajaram and J.C. Kuriacose, 2nd Ed., Thermodynamics for Students of Chemistry – Classical, Statistical and Irreversible, Shobhan Lal Nagin, New Delhi, 1996.
3. G.W.Castellan, Physical Chemistry, Narosa, 1996.
4. K.J. Laidler, Chemical Kinetics, 3rd Ed., Pearson Education, 2004.
5. S. Glasstone, Text book of Physical Chemistry, McMillan, 1974.
6. K.K. Rohatgi – Mukherjee, Fundamentals of Photochemistry, New Age International, 2000.

Reference Books

1. J. Moore, Physical Chemistry, 5th Edn., Orient Longman.1972
2. S. Glasstone, Thermodynamics for Chemists, Affiliated East West Press, 1969.
3. I.M. Klotz, P.M. Rosenberg, Chemical Thermodynamics: Basic Concepts and Methods, 7th Ed., John Wiles & Sons, 2008.
4. A.A. Frost, R.G.Pearson, Kinetics and Mechanism, John Wiley & Sons, 1953.
5. J.I. Steinfeld, J.S.Francisco, W.L. Hase, Chemical Kinetics and Dynamics, 2nd Ed, Prentice Hall, 1999.
6. K.S. Gupta, Chemical Kinetics and Reaction Mechanism , RBSA Publishers, 1992.
7. A.J. Bard, L.F. Pahlkner, Electrochemical methods – Fundamentals and applications, 2nd Ed., Wiley-VCH, 1998.
8. J. Albery, Electrode kinetics, Clarendon Press, Oxford Chemical Series, 1979.
9. D.R.Crow, Principles and applications of Electro Chemistry, Chapman & Hall.
10. D.A. McQuarrie, D. Simon, Physical chemistry, A Molecular Approach, Viva Books Pvt. Ltd, 2003.
11. J.O. Bockris and A.K.N. Reddy, Modern Electrochemistry, 2nd Ed., Springer, 2006.
12. L.I. Anthrapov, Theoretical Electrochemistry, Mir Publishers, Moscow, 1972.
13. P.H. Rieger, Electrochemistry, Prentice-Hall, Inc, 1987.

14. K.K. Rohatgi – Mukherjee, Fundamentals of Photochemistry,New Age International, 2000.
15. N.J. Turro, Molecular Photochemistry, W. A. Benjamin, 1966.
16. J.R. Lakowicz, Principles of fluorescence spectroscopy, Springer, 2006. C.H. Hamann, A. Hammett, W. Vielstich, Electrochemistry, Wiley-VCH, 1998.

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CHE 015E - MEDICINAL CHEMISTRY AND DRUG DESIGN

Unit I Molecular modeling and Computer aided drug design.

Basic features of molecular modeling, Molecular mechanics, *Ab initio*, DFT and semi-empirical methods-Energy minimization; Local and global energy minima, saddle point-Force fields, Monto Carlo simulation; Molecular docking- Molecular Dynamics; Introduction, basic principles, Mechanics and dynamics of Bio-macromolecules.

Stages in drug development-conventional approach-Rational drug design-Target identification-Sequence to structure - Protein structure prediction - Homology modeling-Active sites-Lead structure identification, Target – Substrate Docking - Scoring-molecular descriptors - High throughout screening and combinatorial chemistry-Structure-activity relationship (SAR)– Toxicity, Patents

Unit II Medicinal Bioinorganic Chemistry

Bioinorganic Chemistry of quintessentially toxic metals. Lead, Cadmium, Mercury, Aluminum, Chromium, Iron, Copper, Plutonium. Detoxification by metal chelation. Drugs that act by binding at the metal sites of Metalloenzymes.

Chemotherapy-Chemotherapy with compounds of certain non-essential elements. Platinum complexes in Cancer therapy – Cisplatin and its mode of action – Cytotoxic compounds of other metals – Gold containing drugs as anti-rheumatic agents and their mode of action - Lithium in Pschycopharmocological drugs. Molecular channels and transport processes.

Unit III Medicinal Bioorganic Chemistry

Introduction – Study of drugs – Important terminologies in pharmaceutical chemistry – Classification and nomenclature of drugs – Antibacterial drugs – Sulpha drugs: sulphanilamide,sulphadiazine - Antibiotics: chloraphenicol, penicillin, Analgesics: morphine, heroin, Anticonvulsant: Barbiturates, oxazolindiones, streptomycin, terramycin

Unit IV Vitamins

Structure and function of Vitamins A, B_1, B_2, C, E and H

Unit V Drug Action

Mechanism of action of drugs – Metabolism of drugs – Absorption of drugs, Diabetes: control of diabetes, insulin – Cancer and antineoplastic drugs: antimetabolites, plant products – Cardio vascular drugs: Antiarrhythemic drugs, antihypertension drugs

Text Books

1. Andrew Leach, Molecular Modelling, Principles and Applications, 2nd Ed., Pearson, Prentice Hall, 1991.
2. G.L. Patrick, An Introduction to Medicinal Chemistry, Oxford University, Press, 2nd Ed., 2001.
3. A. R Leach, V. J. Gillet, An Introduction to Chemininformatics, Springer, The Netherlands, 2007.

Reference Books

1. J. Ghosh, Fundamental Concepts of Applied Chemistry, S. Chand and Co., New Delhi, 2006.
2. G. Thomas, Fundamentals of Medicinal Chemistry, John Wiley & Sons, 2003
3. A. Burger, Medicinal Chemistry, I arts I and II, Wiley, N. Y.,1969.

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SEMESTER – II

CHE021C ORGANIC CHEMISTRY – II

Unit I Introduction to stereochemistry

Concept of chirality: specification on configuration by Cahn, Ingold and Prelog system of notation, compounds with more than one chiral centre – calculation of number of stereisomers – erythro and threo nomenclature; interconversions of Sawhorse, Fisher and Newman's Projections.

The concept of prochirality: Topicity and prostereoisomerism – equivalent, enantiotopic and diasteriotopic ligands and faces. Atropisomerism – concept of axial chirality 'R' and 'S' nomenclature of some axially chiral molecules.

Geometrical isomers – E & Z nomenclature determination of configuration of geometrical isomers by physical and chemical methods.

Unit II Conformational analysis of acyclic and cyclic system

Definition – restricted rotation about carbon – carbon single bonds – conformations of ethane and n-butane – conformational free energy – conformational isomers and atropisomers – population of conformers – influence of dipole – dipole repulsion, van der Waals attractive force, intramolecular H-bonding on the stability of conformers.

Conformational analysis of cyclohexane systems – stability and isomerism in mono and di substituted cyclohexane – flexible conformers – conformational analysis of cyclohexane and its derivatives ($A^{1,2}$ and $A^{1,2}$ strain) cyclohexanones – alkyl ketone effect - α - halocyclohexanones – anomeric effect.

Unit III Dynamic stereochemistry conformation and reactivity

Conformation and reactivity in acyclic systems – stereo electronic and steric factors – simple examples illustrating E2 and cis eliminations, intramolecular rearrangements and neighbouring group participation, Curtin-Hammett principle.

Conformation and reactivity in cyclohexanes and decalins – simple reactions illustrating stereo and stereoelectronic factors – esterfication, oxidation, nucleophilic substitution at ring carbons and elimination reactions - reactions involving intramolecular rearrangements – formation and cleavage of epoxides and neighbouring group participation – reactions of enols and enolates.

Unit IV Synthetic Principle and Reagents

Reterosyntheitc analysis – synthons and synthetic equivalents — Chiron's umpolung – protection and deprotection – selectivities (product chemo, regio and stereo)

Use of the following reagents in organic synthesis and functional group transformation – Dicyclohexylcarbodiimide, 1,3 dithiane (reactivity umpolung), trimethylsilyl iodide, tri-n-butyltin hydride, Woodward and Prevost hydroxylation, DDQ Wilkinson's Catalyst – Wittig reaction

Unit V Oxidation and Reduction

Oxidation of organic compounds with reagents based on peroxides, peracids, ozone, oxides of osmium, chromium, ruthenium and silver, dimethyl sulfoxide, iodine and selenium dioxide

Reduction of organic compounds with reagents based on alkali and alkaline earth metals, boron and aluminium hydrides, hydrazine, formic acid and dissolving metals. Clemmenson reaction, Wolf Kishner reduction, Birch Reduction.

Text Books

1. E.L.Eliel, Stereochemistry of Carbon Compounds, McGraw Hill, 1962.
2. V.M.Potapov, Stereochemistry, MIR Publishers, Moscow 1979.
3. D.Nasipuri, Stereochemistry of Organic compounds, 2nd Edn, New Age International, New Delhi, 1972.

Reference Books

4. E.L.Eliel , N.C.Allinger, S.J.Angyal and G.A.Morrision, Conformational analysis, Interscience, New York, 1965.
5. C.Djerassi, Optical Rotatory Dispersion – Application to Organic Chemistry, Mc Graw Hall, 1960.
6. R.E.Ireland, Organic Synthesis, Prentice Hall, 1969.
7. S.Turner, Design of Organic Synthesis, Elsevier, 1976.
8. S.Warren, Designing Organic Synthesis – A programmed introduction to synthon approach, Wiley, New York, 1978.
9. R.K.Makie, P.M.Smith, R.A.Aatkin, Guide book to Organic Synthesis, 2nd Edn., Longman Scientific and Technical, London, 1990.
10. C E Coates. M L H Green, P Powell K Wade Principles of Organometallic Compounds Chapman and Hall, 1977.
11. C E Coates. M L H Green, K Wade. Organometallic Compounds Vol I. Mathew, 1967.
12. J.M.Swan and D.St.C.Black, Organometallics in organic synthesis, Chapman and Hall, London, 1974.

INORGANIC CHEMISTRY - II

CHE022C STUDIES IN COORDINATION CHEMISTRY

Unit I Chemistry of Coordination Compounds

Brief review of the general characteristics of transition elements, nomenclature of coordination complexes, Isomerism in coordination compounds, types of ligands and chelate effect, stepwise and overall formation constants-determination of stability constant by Job's continuous variation method., VB theory and CFT - Splitting of d-orbitals under different geometries – CFSE – evidence for CFSE-factors affecting CFSE – spectrochemical series – Jahn-Teller distortion- application of d-orbital splittings to explain magnetic properties, Limitations of CFT – MO theory – sigma and pi-bonding in complexes – Nephelauxetic effect

Unit II Electronic Spectra of Metal Complexes

Term symbols for atoms and ions – splitting of orbitals and terms in crystal fields – characteristics of d-d transitions – energy levels – Orgel and Tanabe – Sugano diagram – effect of Jahn – Teller distortion and spin-orbit coupling on absorption spectra – crystal field spectra of transition metal complexes – calculation of 10Dq and β for Co(II) (O_h and T_d) and Ni(II) (O_h) complexes- charge transfer spectra of bipyridine and related diimine systems ORD and CD: Chirality and the special nomenclature of chiral coordination compounds - optical activity, ORD and CD – Cotton effect – absolute configurations of chiral coordination compounds

Unit III Inorganic Reaction Mechanism

Electron transfer reactions: Outer-sphere and inner sphere electron transfer reactions – The Marcus theory – non-complementary reactions – synthesis of coordination compounds by electron transfer reactions.

Substitution reactions Trans Effect - theories of trans effect - substitution reactions of square planar complexes of Pt(II) and other d^8 metal complexes – significance of trans-effect – substitution reactions of octahedral complexes – acid and base hydrolysis reactions – anation reactions, the template effect and macrocyclic ligands.

Unit IV Organometallics

The 18 electron rule – applications and limitations – Isolobal concept and its usefulness Hapticity, Metal alkyl and aryls – olefin and acetylene complexes – Zeise salt – Dewar-Chatt approach to bonding in olefins & cyclobutadiene complexes, cyclopentadiene and benzene complexes of transition metals (preparation, bonding and reactions), – Fluxional molecules. Homogeneous catalysis involving organometallics – oxidative addition and

reductive elimination reactions – hydrogenation, isomerization and hydroformylation of olefins – carbonylation of methanol, oxidation of olefins (Wacker process) - heterogeneous catalysis – Ziegler-Natta polymerization of propylene.

Unit V Pi-acceptor Complexes

Synthesis, structure and bonding of mono nuclear and poly-nuclear carbonyls – nitrosyl complexes – dinitrogen complexes – metal carbonylato complexes, carbonyl hydrides and complex metal cyanides.

Text Books

1. J.D. Lee, Concise Inorganic Chemistry, 5th Ed, Wiley, 1999.
2. J.E. Huheey, Inorganic Chemistry, 3rd. Ed., Harper & Row publisher, 1983
3. D.F. Shriver, P.W. Atkins, Inorganic Chemistry, 3rd Ed, 1999

Reference Books

1. D.E. Douglas, D.H. McDaniel, J.J. Alexander, Concepts and Models in Inorganic Chemistry, 3rd Ed. 1994.
2. F.A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry, 4th Ed., John Wiley & Sons,1986
3. S.F.A. Kettle, Physical Inorganic Chemistry – A Coordination Chemistry Approach, Oxford University Press, 1996.
4. A.G. Sharpe, Inorganic Chemistry, Pearson Education, 2008.
5. P. Powell, Principles of Organometallic Chemistry, 2nd Edn., ELBS, 1991.
6. F. Basolo, R.G. Pearson, Mechanism of Inorganic Reactions, 2nd Ed., John Wiley, 1967.
7. N. N. Greenwood, A. Earnshaw, Chemistry of the Elements, 2nd Edn., BH, 1997.
8. M. F. Purcell, J. C. Kotz, Inorganic Chemistry, Saunder, 1977.
9. Oxford Chemistry Primers Series, No.12, M. Bochmann, Organometallics 1: Complexes with transition metal-carbon σ bonds and No. 13

   M. Bochmann, Organometallics 2: Complexes with transition metal- carbon π-bonds.
10. J.P. Collman, L.S. Hegedus, J.R. Nortan, R.G. Finke, Principles and Applications of Organotransition Metal Chemistry, University Science Books, 1980.
11. R. Hoffmann, Angew. Chem. Int. Ed., Engl. 21, 711-800, 1982.

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CHE 024C INORGANIC CHEMISTRY PRACTICALS

Practical – A: Qualitative Analysis

Less common metal ions – Mo, Se, Te, Ce, W, Ti, Zr, Th, U, V, Li (two metal ions in cationic and anionic forms)

Practical – B : Quantitative Analysis

a) EDTA titrations : Zn(II), Mg(II), Cu(II) and Ni(II)

b) Redox titrations : Fe(II) vs. Ce(IV) , Fe(II) vs. dichromate

NO_2^- vs. Ce(IV)

c) Spectrophotometric methods of analysis :

Fe(II), Cu(II) .

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CHE023C PHYSICAL CHEMISTRY - II

Unit I Quantum Theory – I

Planck's quantum theory – Bohr atom model - Wave – Particle duality – Uncertainty Principle – Operators and commutation relations – Sums and product of operator, commutator, linear and non-linear operator, Hermitian and Hamiltonian operator, Postulates of quantum mechanics and Schrodinger equation – orthogonalisation and normality - Free particle – Particle in a box - one and three-dimensional, distortion of the box and Jahn-Teller effect, quantum numbers, zero-point energy, , finite potential barrier – tunneling.

Unit II Quantum Theory – II

Derivation of angular momentum operator, Rigid rotator-Harmonic oscillator. The hydrogen atom – space quantization of electronic orbits – electron spin - Approximate methods of solving the Schrodinger equation – The perturbation and variation methods – Application to He atom - Angular momentum– spin orbit interaction – vector model of the atom – term symbols - Pauli exclusion principle Slater determinant. Atomic Structure Calculation

Unit III Quantum Theory – III

Molecular Orbital and valence bond theory of molecules: The Born–Oppenheimer approximation, MO treatment of H_2^+, and MO and VB treatment of H_2 molecule – comparison of MO and VB methods. Bonding in homo and hetero nuclear diatomics (HF, CO, NO) – polyatomic molecules concept of hybridization -Huckel theory of conjugated systems - application to ethylene, butadiene.

Unit IV Surface Chemistry and Catalysis

Surface Phenomena: Gibbs adsorption isotherm – solid- liquid interfaces – contact angle and wetting – solid-gas interface – physisorption and chemisorption – Freundlich, Langmuir, Temkin, BET isotherms – surface area determination.

Homogeneous catalysis – Acid-base catalysis – Acidity function – Enzyme catalysis – Michaelis–Menten kinetics. Kinetics of surface reactions involving adsorbed species – Langmuir-Hinshelwood mechanism, Langmuir – Rideal mechanism – Rideal –Eley mechanism. Basic aspects of semiconductor catalysis and applications

Solar energy conversion – Photogalvanic cell – Photoelectrochemical cells – Electrolysis of water.

Unit V Polymer Chemistry

Overview of polymers – Structure and classification of polymers – Kinetics and mechanism of free radical and ionic polymerizations - Coordination polymerization, Zeigler–Natta catalysis - Degree of polymerization - Condensation – Self catalysed and Non-catalysd polycondensation, Copolymerization - Equation and significance, Molecular weight of polymers– Determination of molecular weight – Light scattering and viscosity methods - Gel permeation chromatography. Polyesters, silicones, rubbers and fibres.

Text Books

1. A.K. Chandra, Introductory Quantum Chemistry, 4th Ed,. Tata McGraw Hill, 2009.
2. I.N. Levine, Quantum Chemistry, Allyn and Bacon, 1983
3. P.W. Atkins, Molecular Quantum Mechanics, 2nd Edn, Oxford Univ. Press, 1987
4. F.W. Billmeyer, Jr., A Text Book of Polymer Science, John Wiley, 1971.
5. V.R. Gowariker, N.V. Viswanathan, J. Sreedhar, Polymer Science, New Age Publishers, 1986.
6. P.W. Atkins,Physical Chemistry, 7th Ed., Oxford University press, 2002.
7. S. Glasstone, Text book of Physical Chemistry, McMillan, 1974.

Reference Books

1. D.A. McQuarrie, D. Simon, Physical chemistry, A Molecular Approach, Viva Books Pvt. Ltd, 2003.
2. D.A. Mcquarrie, Quantum Chemistry, University Science Books, 1998.
3. F.L. Pillar Elementary Quantum Chemistry, McGraw Hill, 1968.
4. J.P. Lowe and K.A.Peterson, Quantum Chemistry, 3rd Edn., Elsevier 2006.
5. A.W. Adamson, Physical Chemistry of Surfaces, 4th Ed., John Wiley, 1982.
6. B.M.W. Trapnell, Chemisorption, Academic Press, 1955.
7. P.J. Flory, Principles of Polymer Chemistry, Cornell University Press, 1971.
8. A. Tager, Physical Chemistry of Polymers, Mir Publishers, 1978.

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CHE25E Environmental Science, Green Chemistry and Asymmetric Synthesis

Unit I – Water Pollution

Types of water pollution, ground water and surface water pollution – sources and harmful effects – sources and effects of major water pollutants –inorganic pollutants – oxygen demanding wastes - organic pollutants – plant nutrients – detergents – radioactive wastes – nuclear pollution – sources effects of ionizing and non-ionizing radiation.

Unit II – Air Pollution

Atmosphere-structure – functions and photochemical reactions – sources of air pollution- natural and man made – classification and effects of air pollutants – CO, CO_2, SO_2, SO_3,NO and NO_2 – hydrocarbon as pollutant – reactions of hydrocarbons and effects – particulate pollutants – sources and effects of Organic particulate and Inorganic particulate Green House effect – impact on global climate – role of CFC's – ozone holes – effects of ozone depletion – smog-components of photochemical smog-effects of photochemcial smog.

Unit III – Pesticides and Soil Pollution

Pesticides – classification, mode of action – toxic effects of chlorinated hydro carbons, organophosphorous compounds and carbamates – alternatives to chemical pesticides – (pheromones, Juvenile harmones, chemosterilization)

Unit IV – Green Chemistry

Green Chemistry - Definition, principles and requirements, water mediated reactions - solventless reactions – microwave assisted reactions – solid supported reactions – uses of ionic liquids and supercritical carbondioxide reaction in organized media – uses of calixarene, zeolites, cyclodextrin and other supramolecules as media for selection reactions - clay catalysed reactions – definitions and examples of multicomponents reaction and tandem reactions – atom economy reactions.

Unit V – Asymmetric Synthesis

Importance of asymmetric synthesis – problems with resolution methods – optical purity - enantiomeric excess – diastereomeric excess – chiral, substrate controlled, auxillary controlled, catalyst controlled and solvent controlled asymmetric synthesis, example for each case, synthesis of longifolene by EJ Corey method.

Text Books

1. Asim K.Das, Environmental Chemistry with Green Chemistry, Books & Allied (P) Ltd, Kolkata, 2012.
2. B.K.Sharma, Environemtnal Chemistry, Goel Publishers, 2001.
3. J. D. Morrison, Asymmetric Synthesis; Vols 1-5, Academic press, 1983.

SEMESTER – III

CHE031C ORGANIC CHEMISTRY - III

Unit I Organic Photochemistry

Thermal versus photochemical reactions, basic concepts of organic photochemistry, Jablonski diagram – energy transfer mechanism – photochemical reactions of saturated ketones – Norrish type I and II reactions – photoreduction – Paterno - Buchi reaction – reaction of α, β unsaturated ketones – isomerisations – photochemistry of simple olefins – cis-trans isomerisation – di-π methane rearrangement – photochemical oxidations – oxidative coupling – photochemistry of arenes.

Unit II Pericyclic reactions

Definition of pericyclic reactions – electrocyclic, cycloaddition and sigmatropic reactions – selection rules and stereochemistry for thermal and photochemical reactions – explanation on the basis of (i) FMO approach (Fukui), (ii) orbital correlatlion diagram approach (Woodward and Hoffmann) and (iii) aromatic transition state approach (Dewar and Zimmerman) Taking simple systems as example. Diels-Alder reaction, ene reaction, Sommelet – Hauser, Cope and Claisen rearrangements.

Unit III Application of UV, IR and Mass Spectroscopy in organic chemistry

UV spectra – types of excitation or transition probability – chromophores and auxochromes – factors affecting intensity and position of absorption bands – Dienes, Polyenes and Enones – Woodward Fischer rules.

IR Spectra – Hooke's law – factors affecting vibrational frequencies – characteristic group frequencies – Finger print region.

Mass spectroscopy – basic principles – molecular ion peak, parent peak, fragments, metastable peak, isotope peaks – determination of molecular weight and molecular fragment – fragment pattern of simple organic molecules – Mc lafforty rearrangement – Retero Diels Alder reaction.

Unit IV Applications of NMR spectroscopy in organic structural determination

^{1}H NMR spectroscopy – origin of NMR spectra – chemical shift – number of signals – peak areas – multiplicity – geminal, vicinal and long range couplings – factors affecting chemical shifts and coupling constants, first order spectra.

^{13}C NMR spectroscopy: Broadband of offresonance decoupling comparison of ^{1}H and ^{13}C NMR – factors affecting intensity of signals – chemical shifts - γ - gauche effect

Unit V Applications of ESR spectroscopy

ESR electronic Zeeman effect – ESR spectrum of hydrogen atom (first order treatment) – g factors – hyperfine constants – ESR of organic radicals in solution – McConnell's relation – ESR instruments. Structural elucidation using all spectral methods - A problematic approach

Reference Books

1. P.M. Silverstein, F.X. Wester, Spectroscopic Identification of Organic Compounds, 6th Ed., Wiley 1998.
2. J. Mohan, Organic Spectroscopy Principles and Applications, 2nd Ed., CRC, 2004.
3. W. Kemp, Organic Spectroscopy, 3rd Ed., MacMillon, 1994.
4. D.L. Pavia, G.M. Lampman, G.S. Kriz, Introduction to Spectroscopy, 3rd Ed., Brooks Cole, 2000.
5. R.T. Morrison and R.N. Boyd, Organic Chemistry, 6th Ed., Pearson, 1992.
6. J.D. Coyle, Organic Photochemistry, Wiley, 1985.
7. J.M. Coxon, B. Halton, Organic Photochemistry, 2nd Ed., Camb. Univ. Press, 1987.
8. G.R. Chatwal, Organic Phtochemistry, 1st Ed., Himalaya Publications house, 1998.
9. J. Clayden, N. Greeves, S. Warren, P. Wothers, Organic Chemistry, 1st Ed., Oxford University Press; 2000.
10. C.H.Depuy and D.L.Chapman, Molecular Reactions and Photochemistry, Prentice Hall, 1975.
11. T.L.Gilchrist and R.C.Storr, Organic Reactions and Orbital Symmetry, 2nd Edn., Cambridge, 1972.
12. R.E.Lehr and A.P.Marchand, Orbital Symmetry, A problem solving approach, Academic Press, New York, 1972.
13. A.L.Bellamy, An introduction to conservation of orbital symmetry, Longmann, 1975.
14. S.M.Muherjee and S.P.Singh, Pericyclic Reactions, Macmillan, 1976.

CHE032C INORGANIC CHEMISTRY – III

Unit I Infrared Spectroscopy

Spectroscopy in the structural elucidation of simple molecules like N_2O, ClF_3, NO_3^-, ClO^-_4 – effect of coordination on ligand vibrations – uses of groups vibrations in the structural elucidation of metal complexes of urea, thiourea, cyanide, thiocyanate, nitrate, sulphate and dimethyl sulfoxide

Unit II NMR Spectroscopy

Examples for different spin systems – chemical shifts and coupling constants (spin-spin coupling) involving different nuclei (^1H, ^{19}F, ^{31}P, ^{13}C) interpretation and applications to inorganic compounds- NMR spectra of P_4S_3,H_3PO_3,H_3PO_2 and HPF_2. ^{19}F NMR spectra of ClF_3, BrF_3 and equimolar mixture of TiF_6 and TiF_4 in ethanol – Effect of quadrupolar nuclei (^2H, ^{10}B, ^{11}B) on the ^1H NMR spectra, Satellite spectra.

Systems with chemical exchange - study of fluxional behavior of molecules NMR of paramagnetic molecules – isotropic shifts contact and pseudo-contact interactions – Lanthanide shift reagents.

Unit III EPR Spectroscopy

Theory of EPR spectroscopy - Spin densities and McConnell relationship – presentation of the spectrum-hyperfine splitting, Applications of ESR to some simple systems such as CH_3, *p*-benzosemiquinone, Xe_2^+ - Factors affecting the magnitude of g and A tensors in metal species - Zero-field splitting and Kramers degeneracy – Spectra of VO(II), Mn(II), Fe(II), Co(II), Ni(II) and Cu(II) complexes

Mossbauer Spectroscopy

Theory-Doppler effect - isomer shift-quadruple splitting-magnetic hyperfine splitting-application of MB spectroscopy to inorganic compounds

Unit IV Nuclear Chemistry

Properties of nucleus – different types of nuclear forces – liquid drop model, shell model of nucleus – nuclear reactions induced by charged particles – Q value – nuclear reaction cross section, significance and determination – theory of nuclear fission – reactor and its components – production of feed materials for nuclear reactors – disposal of radioactive wastes – nuclear fusion, stellar energy. Application of radioisotopes in agriculture, industry and medicine – neutron activation analysis – hot atom chemistry.

Unit V Inorganic Photochemistry

Elementary ideas on the photosystems I and II - Photochemistry of Cr(III), Co(III) and Ru(II) - coordination compounds – photoaquation – photoanation – photoisomerisation – photo redox reactions – charge transfer photo chemistry – photosensitisation – solar energy conversiuon – photogalvanic cell – splitting of water to evolve hydrogen and oxygen – photochemistry of Pt(II) and Pt(IV) complexes.

Text Books

1. R.S. Drago, Physical Methods in Inorganic Chemistry, 3rd Ed., Wiley Eastern Company
2. K.K. Rohatgi-Mukherjee, Fundamentals of Photochemistry, Tata-McGraw Hill, 1981.
3. E.A.V. Ebsworth, Structural Methods in Inorganic Chemistry, 3rd Ed., ELBS, 1987.
4. Arniger, Nuclear Chemistry

Reference books

1. R.S. Drago, Physical Methods in Chemistry, W. B. Saunders Company, 1992.
2. J. Lewis, R.G. Wilkins, Modern Coordination Chemistry, Inter Science publisher, 1960.
2. K.K. Rohatgi-Mukherjee, Fundamentals of Photochemistry, Tata-McGraw Hill, 1981.
3. Collected readings in Inorganic photochemistry, J. Chem. Edn. 1983.
4. G. J. Ferraudi, Inorganic photochemistry, 1973.
5. A.W. Adamson, E.D. Fleishcer, Concepts in Inorganic photochemistry, 1963.

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CHE033C PHYSICAL CHEMISTRY – III

Unit I Group Theory: Concepts

Elements of symmetry – point group classification of molecules – definition and theorems of group – properties of group with examples - symmetry operations as elements of group – group multiplication table – similarity transformations – sub groups – classes – representation of groups - reducible and irreducible representations – Great orthogonality theorem (derivation and proof excluded) – character table for H_2O and NH_3 molecules – format and significance – direct products and simplified procedure for generating and factoring total representations. Symmetry adapted linear combinations – projection operators.

Unit II Group theory: Applications

Molecular vibrations and their symmetry types in typical molecules – IR and Raman activity – bonding with central atom and formation of hybrid atomic orbitals in molecules such a BF_3, $(PtCl_4)_2CH_4$ – simplification of MO calculations – naphthalene, benzene – symmetries of molecular orbitals and electronic configurations – group theoretical selection rules – vanishing matrix elements selection rules for electronic transitions – electronic spectra of the carbonyl chromophore.

Unit III Spectroscopy – I

General features of spectrum – Experimental techniques – Intensities of spectral lines and linewidths - Rotational spectra - Vibrational spectra – Rotation–Vibration spectra of diatomic and polyatomic molecules – Fermi resonance – Basic concepts of FTIR – Raman spectroscopy – Rotational Raman and vibrational Raman – Resonance Raman and Laser Raman – Electronic spectra of diatomic molecules – Franck-Condon principle – Vibrational and rotational fine structure – Fortrat diagram – Predissociation.

Unit IV Spectroscopy – II

NMR – nuclear spins in a magnetic field – Zeeman effect – Larmor precession – Resonance phenomenon – Block equations – Spin - lattice and spin-spin relaxation times – Nuclear shielding and chemical shift – Spin-spin coupling – Basic principles of FT NMR – Inversion recovery and CPMG sequenced for T_1 and T_2 measurements – NMR instrumentaion.

ESR – Electronic zeeman effect – ESR spectrum of hydrogen atom (first order treatment) - g factors – Hyperfine constants – ESR of organic radicals in solution – McConnell's relation – ESR instrumentation.

Unit V Statistical Thermodynamics

Thermodynamics probability and entropy – Maxwell-Boltzman, Bose-Einstein and Fermi- Dirac statistics and applications, - partition function and entropies for translatinl, rotational, vibrational and electronic motions of monoatomic and diatomic molecules – calculations of thermodynamic functions and equilibrium constants – specific heat of solids – Einstein and Debye theories.

Text Books

1. F.A. Cotton, Chemical Applications of group Theory, 3rd Ed., Wiley Eastern, 2004.
2. R.L. Carter, Molecular Symmetry and Group Theory John Wiley, 1998.
3. C.N. Banwell, E. McCash, Fundamentals of molecular Spectroscopy, 4th Ed., TMH, 2008.
4. B.P. Straughan, S.Walker Spectroscopy Vol.3, Chapman Hall, 1976.
5. G.M. Barrow, Introduction to Molecular Spectroscopy, McGraw Hill, 1964.
6. P.K. Ghosh, Introduction to Photoelectron Spectroscopy, John Wiley, 1989.
7. P.W. Atkins, Physical Chemistry, 7th Ed., Oxford University press, 2002.

Reference Books

1. R.L. Flurry, Jr, Symmetry Groups – Prentice Hall, New Jersy 1980.
2. B.E. Douglas and C.A. Hollingsworth, Symmetry in Bonding and Spectra – An Introduction, Academic Press, 1985.
3. S.F.A. Kettle, Symmetry and Structure, John Wiley & Sons, 1985
4. D.A. McQuarrie, D. Simon, Physical chemistry, A Molecular Approach, Viva Books Pvt. Ltd, 2003.

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CHE034C PHYSICAL CHEMISTRY PRACTICALS

Any twenty experiments out of the following experiments (to be decided by the course teacher):

1. Kinetics – Acid Hydrolysis of Ester – Comparison of strength of acids.
2. Kinetics – Acid Hydrolysis of Ester – Determination of Energy of Activation (E_a).
3. Kinetics – Saponification of Ester – Determination of E_a by conductometry.
4. Kinetics – Persulphate – Iodide Reaction – Determination of order, effect of Ionic strength on rate constant.
5. Polymerization – Rate of polymerization of acrylamide.
6. Distribution Law – Study of iodine – Iodide equilibrium.
7. Distribution Law – Study of Association of Benzoic Acid in Benzene.
8. Study of phase diagram of two components forming simple eutectic.
9. Study of phase diagram of two components forming a compound.
10. Determination of molecular weight of substances by TT measurements.
11. Determination of Critical Solution Temperature of phenol water system and effect of impurity on SCT.
12. Adsorption – oxalic Acid\Acetic Acid on charcoal using Freundlich isotherm.
13. Conductometry – Acid – alkali titrations.
14. Conductometry – precipitation titrations.
15. Conductometry - Displacement titrations.
16. Conductometry – Determination of dissociation constant of weak acids.
17. Conductometry – Solubility product of sparingly soluble silver salts.
18. Verification of Onsager equation – conductivity method.
19. Determination of degree of hydrolysis and hydrolysis constant of a substance.
20. Potentiometric titrations – Acid alkali titrations.
21. Potentiometric titrations – Preciptation titration.
22. Potentiometric titrations – Redox Titrations.
23. Potentiometry – Determination of dissociation constant of week acids.
24. Potentiometry- Determination of solubility product and pKa

Reference Books

1. B.P. Levitt, Ed., Findlay`s practical Physical Chemistry, 9th Ed., Longman, 1985.
2. J.N. Gurtu, R. Kapoor, Advanced Experimental Chemistry, Vol.I, S.Chand & Co., 1987.
3. B. Viswanathan and P. S. Raghavan, Practical Physical Chemistry, Viva Books,2009.

CHE35E ANALYTICAL TECHNIQUES

UNIT I Chromatography – I

HPLC: Introduction – Column Packing Materials – Solvent – Detectors – Recorder – Terms and Definitions used in HPLC analysis and applications.

Gas Chromatography: Introduction – Retention Time – Retention Volume – Efficiency – Career Gases – Preparation of Columns – Solid Supports – Stationary Phases Detectors – Temperature Effect – Quantitative and Qualitative analysis and applications.

UNIT – II Chromatography – II

Gel Permeation Chromatography (GPC) : Introduction – Types of gels – Selection of gels – Gel Preparation – Drying of gels – Packing of the Column Application of the sample – Resolution – Detectors and Applications.

Gas Chromatography Mass Spectrometry (GCMS): Introduction – Separators – Carrier gas – Sample Injection – Analyzer and Applications.

Liquid Chromatography Mass Spectrometry (LCMS): Introduction – Ionization – Belt Interface – Instrumentation and Applications.

Unit III Electroanalytical methods

Amperometry-Principles and applications, amperometric titration with examples-comparison with other titration methods-Basic principles of electrogravimetry

Coulometry: principles- coulometry at controlled potential- coulometry at constant current-coulometric titrations-advantages and applications

Cyclic Voltammetry: Principles and simple analytical applications – Interpretation of cyclic voltammogram.

Unit IV Spectrometry and thermal methods

Atomic absorption spectrophotometer (AAS) - principle, instrumentations and applications- types of interferences. Flame Emisssion spectroscopy (FES) - theory, instrumentation and applications, Difference between AAS and FES. Thermal methods of Analysis- principle, instrumentations and applications of TG, DTA and DSC- thermograms of calcium oxalate and $CuSO_4.5H_2O$

Unit V Surface analysis and XRD

Photoelectron spectroscopy-theory-photo sources-electron analyzers - resolution-assignment of bands-Koopman's theorem - principle, instrumentation and applications of UV, XPS and ESCA, Auger effect

Solid State – Diffraction Studies

Crystallographic point groups – space groups – screw axis and glide plane – seven crystal systems and Bravais lattice –Miller indices- interplanar distances in orthogonal crystal systems – X-ray diffraction studies – powder and rotating crystal methods – systematic absences and lattice types – electron diffraction by gases – principles and measurements – determination of structures – comparison between electron, neutron and X-ray diffraction.

Reference Books

1. D. C. Harris, Quantitative Chemical Analysis, 4th Ed., W. H. Freeman, 1995
2. G. D.Christian & J. E. O'Reily, Instrumental Analysis, 2nd Ed., Allyn & Balon, 1986.
3. P.J. Wheatley, The Determination of Molecular Structure, (Unit V), Oxford University Press, 1968.
4. M.P. Seah, D. Briggs, Practical Surface Analysis by Auger and X-ray Photoelectron Spectroscopy, 2nd Ed., Wiley, 1992.
5. F.Moulder, W.F. Stickle, P.E.Sobol, K.D. Bomben, Handbook of X-ray Photoelectron Spectroscopy, Perkin-Elmer Corp., 1992.

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SEMESTER – IV

CHE041C Chemistry of Natural products and Bioinorganic chemistry

Unit I Proteins, peptides, Nucleic acid, Fats and Lipids

Structure and properties of amino acids and proteins, Zwitterions and purification of proteins

Nucleic acids – nucleotides and nucleosides – structure of purine and pyrimidine bases; Phosphordiester bond, double helical structure of DNA. Structure of RNA (tRNA)

Fatty acids - structure and classification, lipids classification and function (Simple, compound and derived lipids)

Unit II Terpenoids

Classification of terpenoids with examples – isoprene rules – General methods of structural determination of terpenes – structure and synthesis of *alpha*-pinene, cadinene, zingeberene and abietic acid

Unit III Alkaloids

General methods of structure analysis of alkaloids – Hoffmann, Emde and von Braun degradations – Structure and synthesis of quinine, papavarine, atropine, narcotine, reserpine and lysergic acid.

Unit IV Steroids

Types of steroids – structure, stereochemistry and synthesis of cholesterol – Structural features of bile acids – Sex harmones – androsterone, testerosterone, estrone, estriol, estradiol, progesterone - Structure of ergosterol.

Circular birefringence, optical rotary dispersion, circular dichroism – Cotton effect curves – octant rule – axial haloketone rule - Applications of chiroptical properties in configurational assignments.

Unit V Bioinorganic Chemistry

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. Classification of copper proteins and examples - Electron transfer (Cu, Zn) – Blue copper proteins

Metalloenzymes: active sites, carboxy peptidase, carbonic anhydrase, superoxide dimutase, xanthine oxidase, peroxidase and catalase; photosynthesis, water oxidation, nitrogen fixation, nitrogenase; ion pump, metallodrugs.

Text Books

1. I.L. Finar, Organic Chemistry, Vol.II, ELBS 1985
2. S.J. Lippard, J.M. Berg, Principles of Bioinorganic Chemistry, Panima Publishing Company, 1977.
3. Gurdeep R Chatwal,Organic Chemistry Of Natural Products, Volume I , Himalaya Publishing House, 2009
4. L. Stryer, Biochemistry, 4th Ed., W. L. Freeman and Co, New York, 1995.
5. D. L. Nelson, M. M. Cox, Lehninger Principles of Biochemistry, 5th Ed.

Reference Books

1. W. Kaim, B. Schewederski, Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, John Wiley & Sons, 1994.
2. Bioinorganic Chemistry, Chem. Education, 62, No. 11, 1985.
3. G.L. Eichorn, Inorganic Biochemistry, Volumes 1 & 2, 2nd Ed., Elsevier, 1973.
4. J.N.Davidson, The Biochemistry of Nucleic acids, ELBS, 1965.
5. J.L.Simonsen, The Terpenes, Vols 1-4, Academic Press, N.Y. , 1957.
6. K.Nakanishi, Natual Products Chemistry, Vols. I & II, Academic Press, 1975.
7. W.Klyne, The Chemistry of Steriods, Methuen and co., N.Y. 1965.
8. Androsterone and Testosterone: *J. Chem. Soc. Perkin Trans. I,* **1986**, 117-123.
9. Estrone, Estradiol and 2-Methoxyestradiol: *J. Org. Chem.* **2009**, *74*, 6362-6364.

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CHEO42C NANO CHEMISTRY AND SUPRAMOLECULAR CHEMISTRY

Unit I Nanoscience and Nanotechnology

Definition of nanodimensional materials, Classification of Nanomaterials – Significance of surface to volume ratio, Size effects - Importance of Nanomaterials - - Simple examples of unique properties of nanosized materials - Elementary aspects of bionanotechnology - Some important recent discoveries in nanoscience and technology, Applications of Nanomaterials

Unit II Carbon-based Nanomaterials

Carbon: Bonding in Carbon compounds, Discovery of Cubane, Fullerenes: synthesis, chemical reactions and properties, Carbon Nanotubes: Structure of Single-Walled Carbon nanotubes, physical properties of Single-Walled Carbon nanotubes, synthesis of Carbon nanotubes, growth mechanisms, chemical modification of Carbon nanotubes –Diamondoid Nanomaterials: diamondoids, thin diamond films (and other ultrahard substances) – Chemical modification of CVD Diamond

Unit III Growth techniques and Characterization tools of nanomaterials

Introduction – top-down vs. bottom-up technique – Lithographic process and its limitations – Non-lithographic techniques : Sputtering, Chemical Vapour Deposition, Pulsed Laser Deposition, Sol-Gel technique-nucleation and growth processes, Electrodeposition, Scanning Probe Microscopy – General Concept and defining Characteristics of AFM – Electron Microscopy – Transmission Electron Microscopy

Unit IV Supramolecular Chemistry – I

Introduction to Supramolecular Chemistry – definitions – concepts – molecular forces - covalent bonding, ion – ion, ion – dipole, dipole – dipole, hydrogen bonding, cation – π, π-π interactions, van der Waals forces, hydrophobic and solvent effects – Common motifs in Supramolecular Chemistry – Host/Guest Chemistry, cation, anion and neutral molecule binding. Molecular receptors and design principles. Cryptands, cyclophanes, calixarenes and cyclodextrins. Methods for binding constant measurement.

UNIT V Supramolecular Chemistry – II

Nucleic acid structure & molecular recognition - DNA & RNA, Protein – primary, Secondary, tertiary & Quaternary Structure – Protein folding problem – principles of molecular association and organization – SAMs, micelles, vesicles and cell membrane – Supramolecular reactivity and catalysis- Molecular devices and Nanotechnology

Text Books

1. G. Cao, Nanomaterials and Nanostructures: Synthesis, Properties and Applications, Imperial College Press, London, UK, 2004.
2. C.N.R. Rao, A. Muller, A.K. Cheetam (Eds), The Chemistry of Nanomaterials, Vol.1, ao 2, Wiley – VCH, Weinheim, 2004.
3. Supramolecular Chemistry: Concepts and Perspectives by Jean-Marie Lehn, VCH, 1995.
4. Supramolecular Chemistry - Fundamentals and Applications: Advanced Textbook by Katsuhiko Ariga and Toyoki Kunitake, Springer, 2006.

Reference Books

1. G.L.Hornyak, J.Dutta, H.F.Tibbals, A.K.Rao, Introduction to Nanoscience, CRC Press, 2008.
2. Mich Wilson, Kamali Kanengara, Geoff smith, Michelle Simmons and Burkherd Raguk, Nanotechnology Basic Science and Energy Technologies, Overseas press (I), N.D. 2005
3. J. W. Steed, J. L. Atwood, "Supramolecular Chemistry", Wiley, 2000.
4. A Practical Guide to Supramolecular Chemistry by Peter Cragg, Wiley, 2005.
5. Core Concepts in Supramolecular Chemistry and Nanochemistry by Jonathan W. Steed, David R. Turner, and Karl Wallace Wiley, 2007.
6. Supramolecular Chemistry (Oxford Chemistry Primers, 74) by Paul D. Beer, Philip A. Gale, and David K. Smith, Oxford Science Publications,1999.

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