PHDCHEM2A MODERN METHODS OF ORGANIC SYNTHESIS

Unit I

Synthons and Synthetic Equivalents

Introduction to disconnections – Synthons and synthetic equivalents – Electron donors (nucleophiles) – electron synthon approach – Electron acceptors – (electrophiles) – Introduction of functional groups – Regioselective and stereoselective alkylation of cyclic ketones, cyclic enones.
C-alkylation versus O-alkylation: Enamines and selection alkylation (Mono and di) via enamine reactions. Olefination of carbonyl compounds – Wittig reactions, McMurry method.

Retrosynthetic Analysis of Simple Organic Compounds

Antithesis of mono and dofunctional open chain target molecules. Retrosynthetic analysis of monocyclic and bicyclic target molecules.

UNIT II

Reagents for Reduction and Oxidation

Catalytic hydrogenation and dehydrogenation, Reduction with LAH, $NaBH_4$, Tritertiarybutoxy aluminum hydride, $NaCNBH_3$, Tributyltin hydride, Me_3SiCN, Alkali metals for reduction, Reductions with hydrazines. Osmium tetroxide, Sharpless asymmetric epoxidation, Chromyl chloride, Ozone, DDQ, Dioxiranes, Lead tetraacetate, Selenium dioxide, DMSO either with Ac_2O or Oxalyl chloride, Dess-Martin reagent. LDA, Phase transfer catalysis (PTC), Merrifield resin, Baker's yeast

Unit III

Functional Group Interconversions

Modern methods of functional group interconversion involving C=O, CHO, -OH, -SH, -COOH, C=C, NH2, COOR, CONHR functions. Reversible protection of reactive sites.

UNIT IV

Asymmetric Synthesis

Introduction: Basic principles of Asymmetric synthesis – Definition – Stereospecific, Stereoselective – Enanatioselective and diastereoselective.

Asymmetric synthesis using chiral reagents: Chiral organoboranes – Application of chiral organoboranes, Reduction (Ipc_2BCl) and allylation and crotylation reactions, T.S. models; Chiral modification of lithium aluminum hydride, BINAL-H – Application in reduction of prochiral ketones; Oxazaborolidines. T.S. model.

Asymmetric synthesis using chiral auxiliary: Chiral auxiliaries derived from proline, Champhor, Menthol and Other chiral pool sources.

Asymmetric synthesis using chiral catalysts: Asymmetric alkylation and allylation of carbonyl compounds, Chirality amplification: Selected reactions: Keck's allylation, TADDOLs and other privileged ligands.

Asymmetric hydrogenation: Early advances DIPAMP, DIOP and Noyori's BINAP. Jacobson catalyst – Evans catalyst.

UNIT V

Transition Metals in Organic Synthesis

Formation of C-C single bonds: Organolithium reagents, Organomagnesium reagents, Organozinc reagents, Application of Organocopper, Organochromium, Organocobalt and Organopalladium chemistry.

Formation of C-C double bonds: Alkene metathesis reactions using ruthenium complexes.

Textbooks and Reference books

1. R. K. Mackie and D. M. Smith, Guide Book to Organic Synthesis ELBS, 1982.
2. S. Waver, Organic Synthesis, The disconnection approach, John Wiley & Sons, 1982.
3. J. March, Advanced Organic Chemistry : Reactions, Mechanisms and Structure, 5th ed., Wiley, 1996.
4. S. H. Pine, J.B. Hendrickson, D. J. Cram and G. S. Hammond, Organic Chemistry, McGraw Hill, 4th ed., 1980.
5. T. H. Lowry and K.S. Richardson, Mechanism and Theory in Organic Chemistry, Harper and Row, 1976.
6. J. D. Morrison, Asymmetric Synthesis: Vol 1-5, Academic Press, 1983.
7. E. N. Jacobsen, A. Pfaltz,. H. Yamamoto, Eds., Comprehensive Asymmetric Catalysis, Springer 2000.
8. R. Noyori,.Asymmetric Catalysis in Organic Synthesis, Wiley-NY 1994.
9. I. Ojima, Catalytic Asymmetric Synthesis , VCH-NY, Pergamon, 1998.
10. H. B. Kagan, Aymmetric Synthesis, Thieme Medical Publishers, Ist Edn., 2003.
11. W. Carruthers, I. Coldham, Modern Methods of Organic Synthesis, Cambridge University Press, 4th edition, 2004.
12. I. L. Finar, Organic Chemistry, Vol.II, 5th ed., ELBS, 1975.

PHDCHEM2B TECHNIQUES IN ORGANIC SYNTHESIS AND SPECTROSCOPY

Unit I

Synthetic Principle and Reagents

Reterosyntheitc analysis – synthons and Synthetic equivalents — Chiron's umpolung – protection and deproduction – 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-butyl tin hydride, Woodward and Prevost hydroxylation, Osmium tetroxide, DDQ Wilkinson's Catalyst – Wittig reaction, Clemmenson reaction, Wolf Kishner reduction, Birch Reduction.

Unit II

Oxidation and Reduction

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

Reduction of organic compounds with reagents based on alkali and alkaline earth metals, boron, aluminium, hydrogen, hydrazine, formic acid and dissolving metals.

Unit III

Green Chemistry

Definition, principles and evolution of green chemistry. Heterogeneous reaction for green chemistry. Alternative solvents: ionic liquids, super critical fluid extraction, organic synthesis using water resistant Lewis acids. Solvent free reaction: Microwave assisted organic synthesis-the reaction vessel, medium, advantages, limitations and application. The use of ultrasound in organic synthesis: Introduction, instrumentation, types of sonochemical reactions, esterification, substitution, oxidation, reduction.

Unit IV

Spectroscopy I

Nuclear Magetic Resonance Spectroscopy

^{1}H NMR spectroscopy : Chemical shift – number of signals – peak areas – multiplicity – geminal, vicinal and long – range couplings – factors affecting these parameters

^{13}CNMR spectroscopy: Broadband of off-resonance decoupling, comparison of ^{1}H and ^{13}CNMR – factors affecting intensity of signals – chemical shifts - γ - gauche effect
2D NMR: NOESY and COSY, application of ^{1}H NMR & ^{13}C NMR in structure elucidation

Unit V

Mass spectroscopy - basic principles – molecular ion peak, parent peak, fragments, metastable peak, iosotope peaks – determination of molecular weight and molecular fragment – fragment pattern of simple organic molecules – Mc lafforty rearrangement Combined spectroscopy problems involving IR, UV, Mass and NMR.

References

1. S.Turner, Design of Organic Synthesis, Elsevier, 1976.
2. S.Warren, Designing Organic Synthesis – A programmed introduction to synthon approach, Wiley, New York, 1978.
3. R.K.Makie, P.M.Smith, R.A.Aatkin, Guide book to Organic Synthesis, 2nd Edn., Longman Scientific and Technical, London, 1990.
4. C E Coates. M L H Green, P Powell K Wade Principles of Organometallic Compounds Chapman and Hall, 1977.
5. J.March, Advanced Organic Chemistry, 4th Edn. John Wiley, New York,1992
6. P.M. Silverstein, F.X. Wester, Spectroscopic Identification of Organic Compounds, 6th Ed., Wiley 1998.
7. J. Mohan, Organic Spectroscopy Principles and Applications, CRC; 2nd Ed., 2004.
8. W. Kemp, Organic Spectroscopy, 3rd Ed., MacMillon, 1994.
9. D.L. Pavia, G.M. Lampman and G.S. Kriz, Introduction to Spectroscopy, Brooks Cole, 3rd Ed., 2000.
10. H. Gunther, NMR spectroscopy, basic principles, concepts and application in chemistry, John Wiley & Sons, 2nd Ed., 1995.

PHDCHEM2C COORDINATION CHEMISTRY AND ORGANOMETALLIC 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, 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, low spin and high spin complexes, – Site preferences - Limitations of CFT – Ligand field theory – MO theory – sigma – and pi-bonding in complexes – Nephelauxetic effect – The angular overlap model.

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 B for Co(II) (O_h and T_d) and Ni(II) (O_h) complexes. Charge transfer spectra of halide complexes – square planar and tetrahedral complexes – cyanide complexes – di-oxygen and di-sulphur complexs – bipyridine and related dimine systems.

Unit III

Organometallics

Hapticity, ligand classification, synthesis and structure – The 18 electron rule – applications and limitations – Isolobal concept and its usefulness. Metal alkyl and aryls – olefin and acetylene complexes – Zeise salt – Dewar-Chatt approach to bonding in olefins – cyclopentadiene, benzene and cyclobutadiene complexes of transition metals – their preparations, 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.

Pi-acceptor Complexes

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

Unit IV

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.

Unit V

Medicinal Inorganic Chemistry: Contrast enhancing agents for medical diagnostics, theory of MRI imaging, Gd based contrast agents-synthesis and structural features; optical contrast agents-Ag and AuNPs. Metal complexes for radiotherapy, diagnostic radiopharmaceuticals

References

1. J.E. Huheey, Inorganic Chemistry, 3rd. Ed., Harper & Row publisher, 1983.
2. D.E. Douglas, D.H. McDaniel, J.J. Alexander, Concepts and Models in Inorganic
3. J.D. Lee, Concise Inorganic Chemistry, 5th Ed, Wiley, 1999.
4. E.A.V. Ebsworth, Structural Methods in Inorganic Chemistry, 3rd Ed., ELBS, 1987.
5. C E Coates. M L H Green, P Powell K Wade Principles of Organometallic Compounds, Chapman and Hall, 1977.
6. C E Coates. M L H Green, K Wade. Organometallic Compounds Vol I. Mathew, 1967.
7. J.P. Collman, L.S. Hegedus, J.R. Nortan, R.G. Finke, Principles and Applications of Organotransition Metal Chemistry, University Science Books, 1980.
8. M. F. Purcell, J. C. Kotz, Inorganic Chemistry, Saunder, 1977.

PHDCHEM2D BIOINORGANIC CHEMISTRY

UNIT I

Chemical elements essential to life forms, dose- response curve, speciation in biological systems – an overview. Biological ligands for metal ions – Proteins, nucleic acids, carbohydrates. Common metal binding modes to amino acid side chains in proteins, metal binding sites in nucleic acids, porphyrins. Various roles of metals in biology – charge carriers, structural role, triggers, electron transfer, dioxygen transport, enzyme catalysis – a brief introduction.

UNIT II

Metalloproteins -I

Copper proteins – classification, Superoxide dismutase (Cu, Zn). Copper in oxygen transport in some lower animals. Nickel enzyme – Urease. Bioinorganic chemistry of nitrogenase. Zinc containing protein: Zn – finger proteins, carbonic anhdyrase. Vanadium in biology.

Unit III

Metalloproteins-II

Iron proteins: Oxygen transport, Hemoglobin, Myoglobin. Iron – sulfur proteins – metal sites. Cytochrome P 450 – Non heme protein – Methane mono oxygenase. Iron storage – Ferritin. Iron transport – siderophore.

UNIT IV

Medicinal bioinorganic chemistry

Metal – nucleic acid interactions, applications for design of nucleic acid targeted complexes, cis-platin and next generation anticancer drugs. Bioorganometallics as drugs. Medical applications of complexes of Ru, Cu, Au, Li
Detoxification by metal complexation, drugs inhibiting metallo enzymes- typical examples. Complexes of Tc & Gd as contrast agents. Ionophores.

UNIT V

Inorganic pollutants

Cd, Hg, radioactive wastes, various oxides, sulphates, chromates, etc. Environmental bioinorganic chemistry, carbon dioxide in the environment and its management. Biogeochemical cycles, biomineralization.

References

1. Rosette M. Roat- Malone, Bioinorganic chemistry: A short course,2nd ed.,Wiley – jinterscience Publication, John wiley & Sons.
2. Frausto Da Silva, J.R.R.:Williams, R.J.P. The biological chemistry of the elements: The Inorganic chemistry of life, Claderon Press, New York, 1991.
3. S.J.Lippard and J.M.Berg, Principles of bioinorganic chemistry, Pnima Publishing company, New Delhi,1997.
4. www.acs.org
5. www.rsc.org.

PHDCHEM2E X-RAY CRYSTALLOGRAPHY AND SUPRAMOLECULAR CHEMSTRY

Unit I

Solid state-basics

Fundamentals of Crystallography – seven crystal systems and Bravais lattice - point groups – space groups – screw axis and glide plane – Miller indices – interplanar distances in orthogonal crystal systems

Unit II

Solid State – Diffraction Studies

X-ray diffraction study – powder and rotating crystal methods - electron diffraction by gases – – Scattering intensity Vs Scattering angle - principles and measurements – determination of structures – Neutron diffraction by crystals – magnetic scattering and measurement techniques - comparison between electron, neutron and X-ray diffraction.

Unit III

Solid State- X-Ray diffraction

X-ray diffraction studies – sources of X-Rays - systematic absences and lattice types – data analysis for cubic system – X-ray intensities – structure factor – X-ray photography, diffractometers – data reduction

Unit IV

Supramolecular chemistry

Concepts and languages of Supramolecular chemistry – various types of non – covalent interaction C-H…X interactions π-π interaction, non-bonded interactions – various types of molecular recognition – hydrogen bonds –various types of molecular recognition
Hydrogen bonded supramolecular patterns involving water / carbonyl / halide motifs – concepts of different types of synthons based on non-covalent interactions – Supramolecular isomorphism/polymorphism – applications of supramolecular chemistry

Unit V

Metallo -organic Frame Works

Organometallic systems – combinations of different interaction to design molecular rods, triangles, ladders, and networks etc – Interligand hydrogen bonds in metal complexes – Implications for drug design.

References

1. 1. F.A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry, 3rd Ed., Wiley-Eastern Company, 1990
2. E.A.V. Ebsworth, Structural Methods in Inorganic Chemistry, 3rd Ed., ELBS, 1987.
3. R. West, Solid State Chemistry and its Applications, John Wiley & Sons, 1984.
4. L. Smart and E. Moore, Solid State Chemistry - An Introduction, Chapman & Hall, 1992.
5. H. V. Keer, Principles of the Solid State, Wiley Eastern Limited, 1993.
6. K. Chakrabarty, Solid State Chemistry, New Age Publishers, 1996.
7. Clegg, W., Crystal structure determination, Oxford University press, New York, 1998.
8. Lehn, J.M. Supramolecular Chemistry, VCH, Wienheim, 1995.
9. Desiraju, G. R. Crystal Engineering: The Design of Orgnaic Solids, Elsevier, Amsterdam, 1989.
10. Desiraju, G.R. & Steiner, T. The weak hydrogen Bond in Structural Chemistry and Biology: Oxford University press: Oxford, 1999.
11. Jeffrey, G. A. Introduction to Hydrogen Bonding: Oxford University press: New York, 1997.
12. Lehn, J.M. Transition metals in Supramolecular chemistry: John Wiley sons: New York, 1999.
13. Desiraju, R. (2001). Current Science, 81, 1038.
14. Rao, C.N.R. (2001) Current Science, 81, 1030.
15. Journals
    a. Crystal Growth and Design. http://www.pubs.acs.org/journals/cgdefu/index.html
    b. Crystal Engineering Communication

http://www.rsc.org/Publishing/journals/ cgdefu/index.html

PHDCHEM2F ANALYTICAL CHEMISTRY

Unit I
Chromatography

Introduction, classification, TLC, column, gas, ion-exchange chromatography, HPLC,GLC, principle, experimental, application, exclusion (size) chromatography – column packing, theory of size of exclusion chromatography – application of size exclusion chromatography.

Unit II
Electroanalytical methods

Poatentiometric methods: reference electrodes and indicator electrodes. The hydrogen calomel, Ag-AgCl electrodes. The glass electrode – its structure, performance and limitations. Measurement of pH. Potentiometric titrations. Redox and precipitation titrations. Electrogravimetry: principle and method. Determination of Cu. Separation of metals. Conductometry: principle and method. Conductance measurements. Conductometric titrations. Coulometry: principle and method. Coulmetric titrations.

Unit III

Spectrophotometry and calorimetry

Introduction – theory of spectrophotometry and calorimetry – deviations from Beer's law – instrumentation –applications – quantitative analysis

Atomic Absorption Spectroscopy

Principle – difference between AAS and flame emission spectroscopy – instrumentation of AAS – single and double beam spectrometers – applications of AAS.

Photoelectron Spectroscopy

Photoelectron spectroscopy-theory-photo sources-electron analyzers - resolution-assignment of bands-Koopman's theorm-UV, X-Ray photoelectron spectroscopy, Auger effect, applications of ESCA.

Unit IV
Thermal methods of analysis
Thermo Gravimetrics (TG), Differential Thermal Analysis (DTA) and DSC-Principle, working and applications, Thermometric titrations.

Unit V

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 – data analysis for cubic system – 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. E.A.V. Ebsworth, Structural Methods in Inorganic Chemistry, 3rd Ed., ELBS, 1987.
5. R.S. Drago, Physical Methods in Inorganic Chemistry, 3rd Ed., Wiley Eastern Company (Units I, II, III & IV).
6. R.S. Drago, Physical Methods in Chemistry, W. B. Saunders Company, 1992.

PHDCHEM2G CHEMISTRY IN NANOSCIENCE AND TECHNOLOGY

Unit I
Nanoscience and Nanotechnology

Definition of nanodimensional materials - Some historical milestones in the saga of nano forms - Size effects - Importance of Nanomaterials - Classification of Nanomaterials - Simple examples of unique properties of nanosized materials - Elementary aspects of bionanotechnology - Some important recent discoveries in nanoscience and technology.

Unit II
Carbon-based Nanomaterials

Carbon : types of Carbon materials, bonding in Carbon compounds, the Nano perspective – Fullerenes: Fullerene properties, Fullerene synthesis, physical and chemical reactions of Fullerenes – 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 – Nonlithographic techniques : Plasma Arc Discharge, Sputtering, Evaporation, Chemical Vapour Deposition, Pulsed Laser Deposition, Pulsed Laser Deposition, Molecular Beam Epitaxy, Sol-Gel technique, Electrodeposition, other processes - Scanning Probe Microscopy – General Concept and defining Characteristics of AFM – Electron Microscopy – Transimission Electron Microscope

Unit IV
Chemical Interactions at the Nanoscale

Bonding considerations at the nanoscale: background, intramolecular versus intermolecular bonding, types of intermolecular bonding , the nano perspective – electrostatic interactions: ion pair interactions, solvent effects, ion-dipole and dipole-dipole interactions, dative bonds, π interactions – hydrogen bonding:standard hydrogen bonds, C-α-H…O Hydrogen bonds, halogen bonds, hydrogen bonds and living things – Van der Waals Attractions – hydrophobic effect.

Unit V
Inorganic Nanoparticles and Nanoporous Materials

Oxide nano particles – Oxomolybdates – Nano catalysis – Porous silicon – Transition and Non transition metal phosphates.

Nanotechnology in biomedical applications: Drug delivery (polymer therapeutics, drug delivery across the bold brain barrier, dendrimers as drug carriers, hydrogels, micelle system), tissue regeneration, gene therapy, photodynamic therapy, biosensors, quantum dot technology, diagnostic imaging, plant and microbes as nanofactories, antimicrobial effect of nanoparticles.

Nanotoxicology: Nanomaterials relevance to human health, environmental implications, toxicological health effects, relevant parameters in nanotoxicology, risk assessment of nanoparticles.

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. Nanobiotechnology. S. Balaji, MJP publishers, Chennai, 2009.
4. Nanotechnology: A Gentle Introduction to the Next Big Idea. M. Ratner & D. Ratner, Pearson Education, Noida.

PHDCHEM2H BASICS OF METALLIC CORROSION AND MONITORY METHODS

UNIT I

Fundamentals Of Corrosion

Definitions-Types Of Corrosion-Electrochemical Theory(ECT) Of metallic And Metal Alloy Corrosion-Diagrammatical Representation of Rusting and ECT-Global And National revenue Loss due To Corrosion-Calculation Of Metallic Corrosion Rate(CR)-Various Units To Express CR.-Constants Used In CR- Accepted By NACE.

Prevention Of Corrosion

Painting-Galvanisation-Elctroplatting-Corrosion Inhibitors-Organic, Inorganic, Polymers. Nanomaaterials, Green Inhibitors Extracted From Plants And Seawater Species-Mode Of Prevention By Inhibitors-Adsorption-Adsorption Isotherms(Several Types)-Graphical Representation-Interpretation-Chemisorption,Physisorption-Differences-Interpretation Of Type Of Adsorption By Heat Of Adsorption.Thermodynamics Of Corrosion –Kinectics Of Corrosion-Caculation Of $\Delta E_{activation,}$ ΔG,ΔH,ΔS-Interpretations On Corrosion Mechanism- Based On Thermodynamical Data.-Correlation Of Data.

UNIT II

Gravimetric Analysis

Inhibition Efficiency, Calculations Based On Mass Loss Of Metal Coupons-Formulas And Constants Used In Calculations For Mild Steel-Low Crbon Steel-Brass-Titanium-Copper-Aluminium-Stainless Steel-Nickel-Units For Ie And Cr-Surface Coverage-Effect Of Ph,Concentration,Time Of Immersion, On Ie And Cr. Synergism-Definition-Examples-Cacluation-Uses.Statistical Analysis-Anova Test –Significance Of Variences –Synergism Parmeter Calculations.

Immersion Method-Interpretation Of Effect Temperature, Acidity And Alkalinity In Medium-Preparation Of Solution As Normal, Molar, Weight - Percentage,Volume-Percentage,Parts Per million Levels-Conversion Units For The Expression Of Corrosion Rates. Selection Of Inhibitors And Medium.

Unit III

ELECTROCHEMICAL TECHNIQUES –Potentiostatic Polarisation studies-Tafel slopes-Linear polarization –EIS(Electrochemical Impedance Spectroscopy)-Nyquist plots-interpretation. Definition-Corrosion Current(E_{Corr})-Corrosion potential-Inhibition efficiency calculations using these data. Theory Of Electrochemical Corrosion-Prediction Of Thermodynamic And Kinetic Study.

UNIT IV

SURFACE MORPHOLOGICAL TECHNIQUES

XPS-X-ray photon spectroscopy-principle,outline of instrumentation-application of binding energy measurement to analyse corrosion parameters-interpretation of XPS.

FTIR Spectroscopy-instrumentation(elementary idea only) interpretation of functional groups and metal complexes. Applications of AFM (Atomic Force Microscopy),ESCA,,SEM, Optical Microscopy-X-ray Diffraction(Powder method) method-AAS(Atomic Absorption Spectroscopy) in corrosion Testing and corrosion control data analysis.

Suggested Journals for study

Surface Analysis by Auger and X-ray Photoelectron Spectroscopy, D. Briggs and J. T. Grant, Eds., IM Publications, Chichester, 2003 ISBN: 1-901019-04-7

K. Siegbahn, C. Nordling, A. Fahlman, R. Nordberg, K. Hamrin, J. Hedman, G. Johansson, T. Bergmark, S.-E. karlsson, I. Lindgren and B. Lindberg, ESCA: Atomic, Molecular and Solid State Structure by mans of Electron Spectroscopy, AlmqvistsndWiksells, Uppsala, Sweden, 1967

Handbook of X-ray and Ultraviolet Photoelectron Spectroscopy, D. Briggs, Ed., Heyden and Son, London, 1977

http://goliath.inrs-emt.uquebec.ca/surfsci/links.html

Unit V

Suggested Journal Papers

1. Open Journal Of Chemical Engineering And Science, Volume 1, Number 1, May 2014

"Analytic Study Based On Electrical Parameters. Of Corrosion Inhibition Of Steel Pretreated By Phosphate Molar Solutions In Concrete Exposed To Aggressive Environments"By Latefa Sail* , Fouad Ghomari, AbdelhafidKhelidj, AbdelillahBezzar

2. "Investigation Of Carbon Steel Corrosion Inhibition By HydroxamicAcids"Phd Thesis, Abdulmajed R. M. Alagta, supervisor Prof.Dr. Erika Kálmán Budapest University Of Technology &Economics, Department Of Chemical And Environmental Process Engineering 2009.

3. British Journal of Applied Science & Technology 9(3): XX-XX, 2015, Article no.BJAST.2015.267 ISSN: 2231-0843 SCIENCEDOMAIN international www.sciencedomain.org **Corrosion Inhibition of Brass in Industrial Cooling Water Systems** Florina Branzoi1* and Viorel Branzoi.

4.Using of Surfactant Nanostructures as "Green Compounds" in Corrosion Inhibition A. Yousefi and S. Javadian International Journal of Environmental Science and Development, Vol. 5, No. 1, February 2014.

REFERENCES

1. Modern Electrochemistry-volA&B by Bockkaris&Reddy,2004.
2. Intoduction to metallic corrosion-by RajNarayan, Oxford university press, NewDelhi.
3. Electrochemical techniques in corrosion prevention by K.A.Kapoor,ELBs edition,2008.
4. Corrosion by F.Fontanna, Oxford university press,London-2005.
5. Spectrochemical analysis by Silverstein second Wilhem publications
6. OrganicSpectrocopy by Dyer,vB.K.sharma,vArun Paul.
7. www.sciencedomain.org

Journals:

1. Sudhish Kumar Shukla ,Quraishi M A., Corros. Sci. 51 (9) (2009) 1990–1997.

2. Ying Yan., Weihua Li., LankunCai.,BaorongHo., ElectrochimicaActa. 53 (20) (2008) 5953–5960.

PHDCHEM2I ENVIRONMENTAL CHEMISTRY

Unit I

Chemistry of Water and Waste Water

Basic Principles and their significance with special reference to colour, turbidity alkalinity, acidity, chemical coagulation, hardness, water softening, disingection, residual chlorine and chlorine demand, dissolved oxygen, biochemical oxygen demand, chemical oxygen demand, nitrogen, phosphate, sulphate, gas analysis, enzymes, factors affecting enzymic activity, bio-chemistry of carbohydrates, proteins, fats and oils under aerobic and anaerobic conditions, detergents and their degradation, composition and characteristics of sewage.

UNIT II & III

Chemistry of air Pollutants

Introduction, definition, classification of air pollutants, effect of air pollutants on man, materials, animals and plants, ambient air quality standards, harmful concentrations, geographical and meteorological factors in air pollution control, measurement of gas flows, volume, quantity and velocity, methods of sampling, particulate collection by liquid scrubbing, centrifugal spray scrubbers, venturi scrubbers, foam scrubbers: field sampling techniques such as deposition, absorption, filtration, condensation, absorption, adhesion, electrostatic precipitation, thermal precipitation; analysis of air pollutants such as particulates sulphur dioxide, carbon monoxide, oxides of nitrogen, hydrogen sulphide, etc, control measures.

Unit IV

Chemistry of Solid Waste

Chemistry of composting; mechanism involved in the decomposition of organic materials like hemicelluloses, proteins, carbohydrates, food materials, organic insecticides, form wastes, etc., by aerobic and anaerobic processes.

UNIT V

Chemistry of Incineration and Pyrolysis:

Incineration: definition, incineration of solid waste; combustion characteristics of various inorganic and organic materials, heating values – determination of heating values of combustible liquid and solid wastes, air requirements for combustion, fate of trace constituents such as sulphur during incineration; gaseous pollutants; definition of pyrolysis; chemical changes taking place in organic and inorganic materials during pyrolysis; importance of pyrolysis in the solid waste disposal; chemistry of recycling of solid waste; recycling and reuse of materials such as paper, plastic, glass, etc.

References :

1. Sawyer, C.N. and PL. McCarty, 'Chemistry for Environmental Engineers', Mc.Graw Hill, 1978.
2. Stumm, W. And J.J. Morgan, 'Aquatic Chemistry', Wiley Interscience 1972.
3. American Public Health Association inc., New York, 'Standard methods for the examination of water and waste water', 1976.
4. Stern, A.C., 'Air Pollution', Vol. 1,2 and 3, Academic Press, New York 1968.
5. Strauss, W.Ed., 'Air Pollution Control', Part 1,2 and 3, Wiley Interscience, New

York, 1960.
6. Jacobs,M.B., 'Chemical Analysis of Air Pollutants', Interscience, New York, 1960.
7. Ross. R.D., 'Air Pollution and Industry', V.N. Reinhold Co., New York, 1972.
8. Leithe, W. Translated by R.Kenor, 'The Analysis of Air Pollutants', Ann Arbor, 1971.
9. Hagerty, D.J., J.L.Pavoni and J."E.Heer, Jr., 'Solid Waste Management', Van Nostrand Reinhold Co., New York, 1973.
10. Wilsion,D.G.'Hand book of Solid Waste Management', V.R.Nostrand, Reinhold, New York, 1977.

PHDCHEM2J CHEMICAL KINETICS

Unit I

Chemical Kinetics : Methods of determining rate laws; Dependence of rate on concentration; Determination of order and rate constant from experimental data; Integrated rate expressions; Collision theory of reaction rates; steric factor, treatment of unimolecular reactions; Modified collision theory; Transition state theory.

Unit II

Chain reactions; Characteristic experimental features of chain reactions; Identification of a chain reaction; Normal and branched chain reactions; Theory of absolute reaction rates, comparison of results with Eyring and Arrhenius equations, ionic reactions; Salt effect; Mechanisms of photochemical, chain and oscillatory reactions

Unit III

Homogeneous catalysis and Michaelis – Menten kinetics; - Lineweaver-Burk and Eadie plots, Effect of temperature and pH, inhibition effect, transient-phase kinetics, heterogeneous catalysis. Kinetics in the excited electronic states: Jablonskii diagram, Laws of light absorption, kinetics of unimolecular photophysical and photochemical processes, photostationary states, photoisomerisation.

Unit IV

Bimolecular photophysical and photochemical proceses: excimers, exciplexes and sensitisation. Mechanism of fluorescence quenching - Stern - Volmer equation, solar cells, photocatalysis, photosensitization, photo-initiated polymerization, epoxy polymers, photorefractive polymers supramolecules, dendrimers, photochromic compounds, Flash photolysis, Chemistry of vision.

Unit-V

Electrode Kinetics: Metal/solution interface- Dependence of electrochemical reaction rate on overpotential-current density for single step and multi-step processes-Influence of electrical double layer on rate constants. Activation and diffusion controlled processes- Marcus kinetics and quadratic dependence of Gibbs free energies-electron transfer processes involving organic and inorganic compounds. Different types of overpotentials- polarization behavior-Mechanism of hydrogen evolution and oxygen reduction in acid and alkaline media- Experimental methods for elucidation of reaction mechanism.

References:

1. M. R. Wright, *An Introduction to Chemical Kinetics*, John Wiley & Sons, 2005.
2. K. J. Laidler, *Chemical Kinetics,* Harper and Row, 3rd Edition, 1990.
3. J. Raja Ram, and J. C. Kuriacose, *Kinetics and Mechanism of Chemical Transformations*, MacMillan Indian Ltd., New Delhi, 1993.
4. C. Kalidas, *Chemical Kinetic Methods: Principles of Relaxation Techniques and applications,*

New Age International (P), 1996.

Supplementary Reading:

1. Richard I. Masel, *Chemical Kinetics & Catalysis*, Wiley-Interscience; 1stEdition, 2001.
2. K. K. Rohatgi-Mukherjee, *Fundamentals of Photochemistry*, Wiley, New York, 3rd Edition, 2002.
3. M. J. Pilling and P. W. Seakins, *Reaction Kinetics*, Oxford Univ. Press, 2nd Edition, 1996.