SARDAR PATEL UNIVERSITY, VALLABH VIDYA NAGAR
Syllabus of M.Sc. Applied Chemistry, Semester- III
(Effective from Academic Year 2020-21)

PT03CACH21 Applied Inorganic Material

Unit – I Industrial Zeolites and metal organic framework

Industrial Zeolites:MELS (Molecularly Engineered Layered Structures) – pillared layered compounds, clay materials, Zeolites - modified zeolites; aluminophosphates;aluminosilicates, talc, Feldspars, Clathrasils, Zeosils, porosils, micro and meso porous compounds – silica based materials, Hetero and iso-poly acids and their salts.**Metal Organic Frameworks:** Introduction to MOFs, Synthesis of MOFs, Post-synthetic modification of MOFs,Characterization of MOFs, Various application of MOFs.

Unit-II Fertilizersand Metal Clusters

Fertilizers: Classification and role of fertilizers, Manufacture and uses of fertilizer urea, ammonium sulphate, ammonium nitrate, single and triple super Phosphate, potassium chloride and potassium sulphate fertilizers, Biofertilizers.

Metal Clusters: Introduction, Cluster compounds of the main group elements-Alkali metals, Transition metal clusters, Metal carbonyl and halide clusters, Boronhydrides, Carboranes and Metallocarboranes, Cage Compounds of non-metalelements.

Unit-III Glass Industries and Ceramics

Glass Industries: Introduction, Basic raw material of glass, manufacturing, process including chemical reaction, types and properties of glass, annealing of glass.

Ceramics (Clay and clay products): Formation, classification, composition and plasticity of clay and clay products, Efflorescence on bricks. Terracotta ware. Pottery porcelain, other clay products, sanitary wares, porcelain insulators their chemistry and compositions. Refractories-Definition, properties and classification, silica and fire clay refractories.

Unit – IV Protective Coatings, Lubricants

Protective Coatings: Paints: Constituents, functions & mechanism of drying. Varnishes and Lacquers; surface preparation for metallic coatings, electroplating (gold) and electrodeless plating (Nickel), anodizing, phosphate coating, powder coating & antifouling coating. **Lubricants:** Functions of' lubricant, Mechanism of lubrication, Fluid or Hydrodynamic Lubrication, Thin film or Boundary lubrication & Extreme pressure lubrication. Lubricantsfor Extreme ambient conditions and for special applications. Properties of lubricants and tests.

ReferenceBooks:

1. Catalysis and Zeolites: Fundamentals and Applications, J.-L. Guth, H. Kessler, Ed. by Jens Weitkamp, LotharPuppe, 1999, Springer.
2. Advanced Inorganic Chemistry, F.A. Cotton,6thEdn.,G. Wilkinson, C.A. Murillo and M. Bochmann, 1999, Wiley.
3. Metal-Organic Frameworks: Applications from Catalysis to Gas Storage,Ed. by Dr. David Farrusseng, 2011, Wiley-VCH.
4. The Technology of Mineral Fertilizers, I. Molodovan, N. Popovici and C. Chivu, 1969.
5. Cluster Chemistry,Guillermo Gonzalez-Moraga, 1993, Springer- Verlag Berlin HeidelbergGmbH.
6. Applied Chemistry, A.K. Bagavathi Sundry, 2006, MJP Publishers.
7. Industrial Chemistry, B K Sharma, 2000, Goel Publishing House Meerut.
8. Speciality Inorganic Chemicals, Ed.W. E. Thomson, 1996, RSC.

Books for further reading:

1. Zeolites and Catalysis: Synthesis, Reactions and Applications, J. Cejka, A. Corma, and S. Zones, 2010, WileyVCH Verlag GmbH & Co. KGaA.
2. Metal Organic Frameworks as Heterogeneous Catalysts, RSC Catalysis Series, Ed.by James J Spivey, 2013, RSC.
3. Supramolecular Chemistry,F. Vögtle, 1991, John Wiley & Sons, Chichester,
4. Fertilizer Nitrogen: Its Chemistry and Technology,Y.Sauchell, 1964, Reinhold.
5. Metal clusters in Chemistry, P. Braunstein, L.A. Oro, P.R. Raithby, 1999, Wiley-VCH Verlag
6. Shreeve's Chemical Process Industries, George T. Austin, 1984, Mograw Hill Intl.
7. Industrial Chemistry, J. S.Jangwaland A. S.Mathuria, 2008, PragatiPrakashan.
8. Dryden's outlines of Chemical Technology, Gopala Rao and Sitting, 1997, East-West Press.
9. Reigel's Industrial Chemistry, James. A, Kent, 1997, CBS Publishers

PT03CACH22 Applied Organic Chemistry - I

Unit – I MolecularOrbitalTheory (MOT)

Introduction to aromaticity,Aromaticity in benzenoids: alternant and non-alternant hydrocarbon, Huckel's rule, Energy levels of π- molecular orbital and the concept of aromaticity, Calculation of energies of orbital in cyclic and acyclic systems and the stabilities of different systems. Molecular orbital theory, HOMO and LUMO concept, Qualitative application of Molecular orbital theory, interactions between σ and π systems (Hyper conjugation), Density functional theory (DFT).

Unit – II Pericyclic Reactions

Molecular orbital symmetry, Frontier orbitals of -ene and -allyl system,Classification of pericyclic reactions and correlation diagrams,FMO and PMO approach, Electrocyclic reactions, Cycloadditions,Sigmatropic rearrangements, Ene reaction, cope rearrangement,Claisen rearrangement, Cheletropic reaction,other related organic reactions.

Unit – IIIDyes &Non-Textile Uses of Dyes

Introduction to dyes and pigment, Study of various classes of dyes: Acidic azodyesBasic dyes, Vat dyes, Heterocyclic dyes, Reactive dyes, Disperse dyes,Fluorescent brighteners and optical whitening agents, Non – Textile uses of dyes: Dyes in medicine, leather, paper, colour photography and electro photography, food and drugs, cosmetics, displays and laser dyes.

Unit – IV Organometallic Reactions

Synthetic applications,Reactions and Mechanism: Coupling reactions such as Suzuki, Heck, Sonogashira, Stille, Hiyama Coupling reactions, Mcmurry reaction, Kumada coupling, Buchwald–Hartwig reaction, etc.,solving problems based on reaction mechanism, reagents, spectroscopy and stereochemistry.

Reference Books:

1. Advanced Organic Chemistry, Part A: Structure and Mechanisms, F. A. Carey and R.J. Sundberg, 2008, Springer.
2. March's Advanced Organic Chemistry, Reactions, Mechanisms, and Structure, M.B. Smith and Jerry March, 2007, Wiley.
3. Stereochemistry of Organic Compounds: Principles and Applications,4thEdn., 2012, D. Nasipuri, New Academic Science.
4. Organic Photochemistry and Pericyclic Reactions,H. Arora,1998, Anmol Publisher.

5. The Chemistry of Synthetic Dye,K. Venkataraman,1952, Academic Press.
6. Chemistry of Synthetic Dyes and Pigments,H.A. Lubs, 1955, Reinhold Publishing Corporation.
7. Organometallic Chemistry,R.C. Mehrotra and Anirudh Singh, 1991, John Wiley, Chichester.
8. Science of Surface Coating,H.W. Chatfield, 1962, Ernest Benn.
9. Synthetic Dyes,Venkat Raman, 2012, Academic Press.
10. Pericyclic reactions-A Textbook: Reactions Applications and Theory, S Sankararaman, 2005, Wiley-VCH.

PT03CACH23 AppliedPhysical Chemistry

Unit – I Applied Electrochemistry

Electrochemical power sources; Concept, Theoretical background, Fuel cells – classification – chemistry of fuel cells,Importance of fuel cells.Types of fuel cell: Hydrogen-oxygen fuel cells, Hydrocarbon-air fuel cell, Alkaline fuel cells, Phosphoric acid fuel cell (PAFC),Proton exchange membrane fuel cells (PEMFC), Solid oxide fuel cells, Molten Carbonate Fuel Cell (MCFC), Solid Polymer Fuel Cell (SPFC), Electrochemical energy conversion: Ag – Zn cells, dry cells, Batteries- lead acid, Ni-Cd and lithium ion-fuel cells,Variousapplications of fuel cell.

Unit – II Energy Systems

Introduction, Alternative energy needs and option, Fossil fuels: petroleum, natural gas and coal – origin, processing production of value added products – available current conversion technologies.Solar Energy conversion devices – photovoltaic cells – photoelectrochemical cells – semiconductor electrolyte junctions, Design and mechanism of solar cells, Silicone solar cells and alternatives, thin film solar cells and third generation solar cells, Thermodynamics limit of light concentrators, Thermodynamics of light conversion.

Unit – III Surface phenomenon and catalysis

Surface Phenomenon & Physical and Colloidal Chemistry of Surfactants

Adsorption-Surface tension, Capillary action, Kelvin equation, Types of adsorption and adsorption isotherms, Measurement of surface area of adsorption, Adsorption of solid from solution, Application of adsorption, Some recent advances in surface physics: Solid interfaces, Liquid interfaces, Liquid – Liquid interfaces, Solid – Liquid interface.

Catalysis

Catalysis-Catalysis choice with respect to reaction velocity, selectivity and economics, Heterogenized homogenous catalysis, catalysis by supported metal ion and metal complexes shape selective catalysis, solids acid catalysts for automobile emission control, Catalysts used in well-known reactions, Catalyst deactivation and reactivation catalysts for future.

Unit – IV Liquid Crystalline Materials

Introduction, Thermotropic&Lyotropic liquid crystals, structure and property relationship, Smectic, nematic& cholesteric liquid crystals, globular and discotic liquid crystals, liquid crystalline polymers.Applications of liquid crystals in chemistry, electronics, medicine and non-destructive testing.Basic chemistry in Ionic liquid, Liquid crystal and Organic ionic plastic crystal.

ReferencesBooks:

1. Principles and Application of Electrochemistry,3rdEdn.,D.R. Crow, 1988, Chapman and Hall.
2. Chemical Application of Group Theory**,**3rdEdn.,Cotton F.A., 2003, Wiley.
3. Surfactants and Interfacial Phenomena, M. J. Rosen, 1978, John Wiley & Sons Inc.
4. Solvent Properties of Surfactant Solutions, K. Shinoda, 1967, Marcel Dekker Inc.
5. Liquid Crystals,S. Chandrasekhar, 1992, Cambridge University Press.
6. Physical Chemistry,8thEdn.,P. Atkins and J. De Paula,2006, W.H.Freeman & Co.
7. Physical Chemistry,G. K. Vemulapalli, Prentice, 1993, Hall of India.

Books for further reading:

1. Surface Active Agents and Detergents, Anthony M. Schwartz and James W. Perry, 1958, Interscience Publishers.
2. Liquid Crystals and Plastic Crystals,Ed. P.A. Winsor and G.W. Gray, 1974, John Wiley & sons.
3. Physical Chemistry,K.J.Laidler, J.H.Meiser and B. C. Sanctuary, 2003, Houghton Mifflin Company.

PT03CACH24 Advanced Practical - I

1. Synthesis and characterization of heterocyclic scaffolds (which cover one pot synthesis, example for concept of protection/deprotection groups, optimization of various reaction conditions, role of catalyst & green chemistry approach etc.). **(min. 2 compounds)**
2. Synthesis and characterization of heterocyclic scaffolds and metal complexes. **(min. 2 compounds)**
3. Characterization of synthesised compounds using various instrumental methods.
4. Synthesis of Urea-Formaldehyde resins and identify % free formaldehyde from the synthesized resin.
5. Synthesis of Phenol -Formaldehyde resins and identify % free formaldehyde from the synthesized resin.
6. Synthesis of Melamine -Formaldehyde resins and identify % free formaldehyde from the synthesized resin.
7. Interpretation of the following spectral technique towards structure elucidation of organic compounds. Mass spectroscopy, UV-Vis Spectroscopy, Infrared spectroscopy, ^{1}H-NMR Spectra, ^{13}C-NMR Spectra, pXRD (Polymorphism 2Θ).
8. AAS – problems based on concepts.
9. Thermal analysis – TGA, DTA, DSC. Problems based on calculation of weight loss, identification of endotherms, exotherms, interpretation of thermograms.
10. Chromatographic methods of analysis – HPLC, GC. Problems based on basic concepts, retention time, progress of reactions, % yield etc.
11. Qualitative analysis of hydrophobic drugs by liquid chromatography mass spectroscopy method (LCMS).
12. Elemental analysis and quantitative determination of sediment using elemental analyzer.

PT03CACH25 Advanced Practical - II

1. Determination of Saponification value of anoil.
2. To determine the percentage of calcium carbonate in a given toothpastesample.
3. Determine the Reichert-Missal value (R. M value) and P.V value of givensample.
4. To determine neutralization capacity of given antacid tablets.
5. To determine free fatty acid in crude and refined edible oil.
6. To determine the total phosphorous as P_2O_5indetergent.
7. Determination of Iodine value of an oil by Wij'smethod.
8. To determine % purity of given alcohol sample by iodometrictitration.

9. To determine the malathion content in a given WDP malathionsample. (WDP: water dispersible powder)
10. To determine % Fe in iron tablet bycolorimetry.
11. To determineNO_3^- nitrogen in water.
12. To determine % of protein in a given sample of milk.
13. Determination of milk adulteration by Conductivity Measurement.
14. Determination of crystallizing point of given Naphthalene balls.
15. To determine total iodine (in ppm) content in given table salt sample.
16. To determine % of Vitamin C in given tablet/Lemon juice.
17. To determine oxidizing powder of commercial hydrogen peroxide solution and analysis of commercial hypochlorite.
18. Determination of moisture content of given sample by Karl-Fischer Titrator.
19. Determine the nature of the complexes formed in the system Ni(II)/Cu(II)/Fe(III) ethylene diamine in water.
20. Determine the composition of the complexes formed in the system Ni(II)/Cu(II)/Fe(III) ethylene diamine in acidic medium pH-2 by slope ratio method.
21. Determine the stability constant of the complexes formed in the system Ni(II)/Cu(II)/Fe(III) ethylene diamine by Job's method of continuation variation.
22. Determine spectrophotometrically the pK value of an indicator (the acid dissociation constant of methyl red.
23. Determination of concentration of cobalt and chromium in a given mixture of the sample.

PT03EACH21 Fundamentalsof Polymer Chemistry

Unit – I Introduction

Basic concepts: Oligomer, Monomer, Polymer, Polymerization and Functionality, Repeating unit, Degree of polymerization, Bonding in polymers, Notation and nomenclature of polymers, Classification of polymers, Types of polymerization, Properties of polymers: mechanical, chemical, thermal, electrical and optical, Examples of polymers –organic and inorganic polymers.

Unit – II Molecular Weight Concepts and Measurement of Molecular Weights

Number average and weight average molecularweights, Molecular weight and degree of polymerization,Polydispersity and molecular weight distribution in polymers, Practicalsignificance of polymer molecular weight, Measurement of molecular weight: End group analysis,Colligative property methods, Freezingpoint depression (Cryoscopy), Boiling point elevation (Ebullioscopy),Membrane osmometry, Vapour phase osmometry,

Viscometry,Dilute solution viscosity, Light scattering, Ultracentrifugation and Gel permission chromatography (GPC)**.**

Unit – III Structure and Properties of Polymer

Order in crystalline polymers - Configurations of polymer chains,Polymer crystal structure and physical properties -crystallization and melting,melting points of homogeneous series, Effect of chain flexibility and other steric factors, Entropy and heat of fusion, Glass transition temperature, Relationship between $T_m$and $T_g$effects on molecular weight.

Unit – IV Techniques of Polymerization

Bulk – solution – suspension and emulsion polymerization, Melt polycondensation, solution polycondensation, Interfacial condensation, Solid and gas phase polymerization, Salient features of different polymerization techniques, Kinetics of polymerization - free radical polymerization, ionic polymerization, condensation polymerization, emulsion polymerization.

Reference Books:

1. Polymer Chemistry – An Introduction, Malcom P. Stevens, 1999, AddisonWesley Publishing Co. Inc. Massachusetts.
2. Introduction to Polymer Chemistry**,** R. B. Seymour, 1971, McGraw – Hill.
3. Polymer Science**,** V. R.Gowariker, N. V. Viswanathan and JayadevSreedhar, 1986, NewAge International.
4. Principles of Polymer Chemistry,2nd Edn.,A. Ravve, 1995, Springer Science-Business Media New York.
5. Principles of Polymers Systems, F. Rodriguez, 1989, Hemisphere Publishing Corporation
6. Principles of Polymer Science,2nd Edn.,P. Bahadur and N. V. Sastry, 2012, Narosa Publishing House.
7. Principleof Polymer Chemistry, P. J. Flory, 1953, Ithaca Press.

Books for further reading:

1. Polymer Chemistry, C. Carraher, Marcel Dekker,1992, Inc., New York-Basel.
2. Textbook of Polymer Science**,** F. W. Billmeyer, 1962, Wiley – Interscience, New York
3. Introduction to Polymers,3rd Edn.,R. J. Young and P. A. Lovell, 2011, CRC Press.
4. Polymers as Aids in Organic Chemistry,Mathur, Narang and Williams, 1980, Academic Press.

PT03EACH22 Drug Design and Application

Unit - I Drug Design

Drugs: Concepts of drug design, Approaches to lead discovery, Combinatorial chemistry,Pro-drugs,Procedures followed in drug design, Concepts of lead compound and leadmodification, concepts of prodrug and soft drugs, structure-activity relationship (SAR), factors affecting bioactivity. Theories of drug activity: occupancy theory, rate theory, inducedfit theory.

Unit-II Introduction to Medicinal Chemistry and Pharmacokinetics

Drug administration, Drug absorption, Drug distribution, Drug Metabolism (general pathway of drug metabolism: Oxidative, reductive and hydrolytic reactions). Drug excretion, elimination using pharmacokinetics parameters in defining drug disposition and in therapeutics, uses of pharmacokinetics in drug development process. Time course of drug action: First order and zero order. Time course of drug concentration change in plasma,Plateau effect.

Unit-III Pharmacodynamics

Receptors, Chemical messengers, Binding sites. Receptor types and subtypes (protein receptors, DNA receptors with examples of Agonists and Antagonists).

Unit - IV Role of FDA in Pharmaceutical Industries

Concept and role of FDA, Substandard Drugs, Introduction and Development ofnew Drugs-Selection of Area, Phase I, Phase II. Phase III Application to FDA for formulation and marketing for new drug. Stability studies and Shelf life fixation.

Reference Books:

1. Burger's Medicinal Chemistry, 4thEdn., Ed. M.E. Wolff, 1979, John Wiley & Sons.
2. Principles of Medicinal Chemistry,2ndEdn.,W.O. Foye, 1981, lea and FebigerPhiladephia.
3. An Introduction to Drug Design, S. N.Pandeya, J. R.Demmock, 1997, New age International Publishers.
4. Introduction of Pharmaceutical II, A. K. Gupta, S. S. Bajaj, 2007, CBS Publishers and Distributors.
5. Computer and their Application to Chemistry, Ramesh Kumari, 2002.Narosa Publishing House.

Books for further reading:

1. The Organic Chemistry of Drugs Synthesis, Daniel Lednicer and L N Mitscher, 1929, John Wiley & Sons.
2. A Text Book of Synthetic Drugs, 4th Edn.,O. D. Tyagi M. Yadav, 1998, Anmol Publication
3. Biopharmaceuticals & Pharmacokinetics, 3rd Edn., D.M. Brahmankar, Sunil B. Jaiswal, 1995, VallabhPrakashan
4. Computer for Chemists, Sudhir K. Pundir, Anshu Bansal, 2010, PragatiPrakashan.
5. ICH guideline for quality (Q) "www.ich.org › page › quality-guidelines"

PT03EACH23 Advanced Computational Methods in Chemistry

Unit – I Computation &Modelling

Introduction to UNIX and WINDOWS, MS - office, MS - Word,MS - Excel,softwares for chemical structure preparation, principles of programming, Algorithm and flow charts. Theory, Liner fitting, Non-linear fitting and equations, Computation &modelling‐ definition of terms; need of approximate methods in quantum mechanics; Computable quantities ‐ structure, Potential energy surfaces and chemical properties; cost and efficiency ‐ relative CPUtime, Software and hardware; Classification of computational methods.

Unit – II Computer Simulation Methods - I

Introduction - Molecular Dynamics (MD) and Monte Carlo method, Calculation of simplethermodynamic properties; energy, heat capacity, pressure and temperature, Phase space, Practical aspects of computer simulation, Periodic boundary conditions, Monitoringthe equilibration, Analysing the results of a simulation, Error estimation.

Unit – III Computer Simulation Methods – II

Molecular Dynamics (MD) method ‐ Molecular Dynamics using simple models ‐MD with continuous potentials, Finite difference methods, Choosing the time step, Setting up and running aMD simulation; Monte Carlo (MC) method – calculating properties by integration, Metropolis method, Random number generators, MC simulation of rigid molecules.

Unit – IV *Ab intio*Methods in Computational Chemistry

Review of Hartree-Fockmethod for atoms, SCF treatment of polyatomic molecules; Closed shell systems - restricted HF calculations; Open shell systems-ROHF and UHF calculations; Roothan-Hall equations, Koopmans theorem, HF limit and electron correlation, Introduction to electron correlation (Post-HF) methods.

Reference Books:

1. Essentials of computational Chemistry: Theories and models, C. J. Cramer,2002, John Wiley & Sons.
2. Introduction to Computational Chemistry, Frank Jensen, 1999, John Wiley &Sons LTD.
3. Computer and their application to Chemistry, R Kumari, 2008, Springer.
4. Computational Chemistry- A Practical Guide for Applying Techniques to Real-World Problems, David Young, 2001, Wiley-Interscience.
5. A Chemist's Guide to Density Functional Theory, W. Koch, M.C. Holthausen, 2000, Wiley-VCH Verlag.
6. Computational Chemistry-An introduction to numerical methods, A.C. Norris, 1981, John Wiley & sons Ltd.
7. Microcomputer Quantum Mechanics, J.P. Killngbeck, 1983, Adam Hilger.

Books for further reading:

1. Exploring Chemistry with Electronic Structure Methods, J. Foresman&Aelieen Frisch,2000, Gaussian Inc.
2. Computer for Chemists,S. K. PundirandA. Bansal, 2010, PragatiPrakashan.
3. Computer and Commonsense, R. Hunt and J. Shelley, 1979, Prentice Hall.
4. Computers in Chemistry, K.V.Raman, 2003, Tata McGraw-Hill Publishing Co. Ltd.
5. Computer Applications in Chemistry, K. Arora, 2004, Anmol Pub.
6. An Introduction to Digital Design,4thEdn., V. Rajaraman and T. Radhakrishnan, 2005, Prentice Hall