ALAGAPPA UNIVERSITY, KARAIKUDI NEW SYLLABUS UNDER CBCS PATTERN (w.e.f. 2017-18)

M.Sc., CHEMISTRY – PROGRAMME STRUCTURE

Sem	Course Code	Name of the Course	Cr.	Hrs./ Week	Marks		
					Int.	Ext.	Total
I	7MCH1C1	Core – I – Organic Chemistry - I	5	5	25	75	100
	7MCH1C2	Core – II – Inorganic Chemistry – I	5	5	25	75	100
	7MCH1C3	Core – III – Physical Chemistry – I	5	5	25	75	100
	7MCH1P1	Core – IV – Inorganic Practical – I	5	10	40	60	100
	7MCH1E1/ 7MCH1E2	Elective– I–A)Applied Chemistry (or) B) Polymer Chemistry	4	5	25	75	100
		Total	24	30			500
II	7MCH2C1	Core – V – Organic Chemistry – II	5	5	25	75	100
	7MCH2C2	Core – VI – Inorganic Chemistry – II	5	5	25	75	100
	7MCH2C3	Core – VII – Physical Chemistry – II	5	5	25	75	100
	7MCH2P1	Core – VIII – Organic Practical – I	5	10	40	60	100
	7MCH2E1/	Elective–II-A) Environmental					
	7MCH2E2	Chemistry (or) B) Computer in	4	5	25	75	100
		Chemistry					
		Total	24	30			500
III	7MCH3C1	Core – IX – Organic Chemistry – III	5	5	25	75	100
	7MCH3C2	Core – X – Inorganic Chemistry – III	5	5	25	75	100
	7MCH3C3	Core – XI – Physical Chemistry – III	5	5	25	75	100
	7МСН3Р1	Core – XII – Physical Chemistry Practical – I	5	10	40	60	100
	7MCH3E1/ 7MCH3E2	Elective—III-A)Pharmaceutical Chemistry (or) B) Material Chemistry	4	5	25	75	100
		Total	24	30			500
IV	7MCH4C1	Core – XIII – Instrumental Methods of Analysis	5	5	25	75	100
	7MCH4E1/	Elective – IV-A) Nano Chemistry (or)	4	5	25	75	100
	7MCH4E2	B) Corrosion Chemistry	4	<u> </u>	25	75	100
	7MCH4E3/	Elective–V-A) Green Chemistry (or)	4	5	25	75	100
	7MCH4E4	B) Molecular Photochemistry	-				
	7MCH4PR	Core-XIV-Project	5	15	25	75	100
		Total	18	30			400
		Grand Total	90	120			1900

M.Sc. CHEMISTRY

I YEAR – I SEMESTER COURSE CODE: 7MCH1C1

CORE COURSE-I-ORGANIC CHEMISTRY-I

Objectives:

- > To impart a knowledge of Electron Displacement.
- ➤ To be familiar with the details of Stereochemistry, Aromaticity and detailed study of aliphatic nucleophilic substitution.

Unit I: Electron Displacement

[15 hrs]

Inductive and Field Effects – Bond Distance – Bond Energies – Delocalized Bonds – Cross Conjugation – Steric Inhibition of Resonance – Hyper Conjugation – Effects of Structure on the Dissociation Constants of Acids and Bases.

Quantitative Treatment of the Effect of Structure on Reactivity – The Hammett Relationship – Significance of Reaction and Substituent Constants – Application of the Hammett Equation in Reaction Mechanism – Limitations, Modification and Deviations – Taft Equation.

Unit II: Stereochemistry

[15 hrs]

Symmetry Elements and Point Group Classification – Conditions for Optical Activity – Optical Isomerism – Definitions – Newmann, Sawhorse and Fisher Projection Formulae – Concept of Chirality – The Cahn-Ingold-Prelog System of Nomenclature – Enantiotopic and Diastereotopic Atoms, Groups and Faces – Molecules with more than One Chiral Centre – Molecular Dissymmetry – Optical Activity of Biphenyls, Allenes and Spirans – Optical Isomerism of Nitrogen and Sulphur Compounds – Asymmetric Synthesis – Cram's Rule.

Geometrical Isomerism:

E-Z Nomenclature – Determination of Configuration of Geometrical Isomers Using Physical and Chemical Methods.

Unit III: Aromaticity

[15 hrs]

Aromatic Character in Benzene, Six – Membered Rings, Five, Seven and Eight Membered Rings – Huckel's Rule and Craig's Rule – Concept of Homoaromaticity and Antiaromaticity – Systems with 2, 4, 8 and 10π Electrons – Systems with more than 10π Electrons – Alternant and Nonalternant Hydrocarbons. Chemistry of Cyclopentadienyl Anion – Fulvene – Azulene –Sydnones. (12), (14), (16), (18) – annulenes. Nomenclature of Bicyclic Systems.

Unit IV: Introduction to Reaction Mechanism

[15 hrs]

Reactive Intermediates – Free radicals – Carbenes – Carbanions – Carbocations – Formation and Stability of Reactive Intermediates – Principle of Microscopic Reversibility – Hammond Postulate.

Aromatic Electrophilic Substitution – Orientation – Reactivity – Mechanism of Nitration, Friedel – Craft's Reaction – Ortho/Para Ratio

Aromatic Nucleophilic Substitution Reactions – S_NAr, S_N1 and Benzyne Mechanisms.

Unit V: Aliphatic Nucleophilic Substitution and Elimination

[15 hrs]

Aliphatic Nucleophilic Substitution: Nucleophilicity and basicity $-S_N{}^1$ and $S_N{}^2$ mechanism – Effect of substrate structure – effect of reaction medium – effect of leaving group – ambident nucleophile – ambident substrates – symphoria – Neighbouring group participation of n, π and σ electrons – $S_N{}^i$ mechanism – Nucleophilic substitution at allylic carbon and vinyl carbon

Elimination: α – elimination, β – elimination – E1, E2 and E1CB mechanism – stereo chemistry of elimination – orientation of double bond – Pyrolytic cis elimination – Bredt's rule.

Books for Reference:

- 1. Finar I.L., Organic Chemistry, Vol. II, 5th Edition, ELBS, England, 1975.
- 2. Morrison R.T., and Boyd R.N., Organic Chemistry, Prentice–Hall, 6th Edition, New Delhi, 1995.
- 3. Ferguson L.N., The Modern Structural Theory of Organic Chemistry, Prentice-Hall, 1969.
- 4. Gould E.S., Mechanism and Structure in Organic Chemistry, Henry Holt and Co., New York, 1959.
- 5. Jerry March, Advanced Organic Chemistry, 6th Edition, Wilely, New York, 2002.
- 6. Lowry T.H., and Richardson K.S., Mechanism and Theory in Organic Chemistry, ELBS, New Delhi, 1995.
- 7. Pinc H., Hendrickson J.B., Cram D.J., and Hammond G.S., Organic Chemistry, 4th Edition, McGraw–Hill Kogakusha Ltd., Tokyo, 1980.
- 8. Shorter J., Correlation Analysis in Organic Chemistry, Clarendon Press, Oxford, 1973.
- 9. Sykes P., Guide Book to Mechanism in Organic Chemistry, 6th edn, Pearson, 2002.

I YEAR – I SEMESTER COURSE CODE: 7MCH1C2

CORE COURSE-II-INORGANIC CHEMISTRY-I

Objectives:

- Z To enable the learners to understand the Ionic bonding, bond properties.
- Z To understand the basic concepts of main group elements, and solid state chemistry.

Unit I: Chemical Periodicity

[15 hrs]

Ionic radii – covalent radii – Vander Waals Radius – bond length, bond order, bond energy, bond polarity – partial ionic character of covalent bonds – electro negativity – electron affinity – Lattice energy – Born-Lande equation-Born Haber cycle – Covalent character in ionic compounds – Fajan's rule - different types of electrostatic interactions – hydrogen bonding. Calculation of ionic radius – Pauling's method and Linde's method. Effective nuclear charge – Slater's rule.

Unit II: Nature of chemical bonding

[15 hrs]

Valence bond theory – hybridisation – quantum mechanical treatment for sp, sp², sp³ hybridisation – Molecular orbital theory – MO theories to the structure of homonuclear (H₂, B₂, C₂, N₂) and heteronuclear (CO, NO, HCl, HF) diatomic and selective polyatomic molecules (CO_3^{2-} , NO₂, BeH₂, CO₂), comparison of VB and MO theories. VSEPR theory and its applications to H₂O, NH₃, IF₅, IF₇, ClO₄⁻ ions, like Xenon halides and xenon oxides.

Unit III: Acid-base systems and non-aqueous solvents

[15 hrs]

A generalized acid base concepts – steric effects and solvation effects – Measures of Acid – Base strength –Factors affecting the strength of acids and bases – common ion effect and Henderson's equation – Hard and Soft acids and bases – symbiosis – theoretical basis of hardness and softness.

Classification of solvents – properties of ionizing solvents. Typical reactions in non – aqueous solvents – liquid HF, Hydrogen cyanide, Sulphuric acid and acetic acid.

Unit IV: Main Group Chemistry

[15 hrs]

Chemistry of borazines and boron nitrides – chemistry of silicon – silanes, higher silanes, multiple bonded systems, disilanes and silicon nitrides.

P-N compounds, cyclophosphazanes and cyclophosphazenes – S-N compounds – S_2N_2 , S_4N_4 , (SN)x, polythiazyl S_xN_4 compounds, S-P compounds – molecular sulphides such as P_4S_3 , P_4S_7 , P_4S_9 and P_4S_{10} .

Unit V: Solid state chemistry

[15 hrs]

Defects in crystal – different types of defects – line and plane defects – stoichiometry and non- stoichiometry defects and effects of defects on physical properties – types of solids – electronic structure of solids – free electron and band theories. Electrical conductivity and superconductivity – High temperature superconductivity – types of Semi-conductors - semiconductors in solar energy conversion.

Books for Refernce:

- 1. H.J.Emelius and Sharpe, Modern aspects of Inorganic chemistry, Universal Book Stall, New Delhi, 1989.
- 2. J.E.Huheey, E.A. Keiter and R.L. Keiter, Inorganic Chemistry Principles of structure and reactivity, 4th edition, Pearson Education, 2002.
- 3. F.Basolo and R.G.Pearson, Mechanism of Inorganic Reactions, Wiley Eastern, 1967.
- 4. K.F.Purcell and J.C Koltz, An Introduction to Inorganic Chemistry W.B. Saunders Company, Philadelphia, 1980.
- 5. P.W.Atkins, D.KShriver and C.H.Langfood, Inorganic Chemistry oxford ELBS, U.K 2009
- 6. H.V. Keer, Principles of the Solid State, Wiley Eastern Ltd., 1993.
- 7. B.R.Puri and L.R.Sharma and K.C.Kalia, Principles of Inorganic Chemistry, Milestone Publishers, New Delhi 2008.
- 8. G.S.Manku, Inorganic Chemistry, TMH Co., 1984.
- 9. F.A Cotton and G. Wilkinson, "Advanced Inorganic Chemistry", 5th Edn, John Wiley & Sons Singapore 1998.
- 10. O.H. Mathur and D.P Tandon, Chemistry of rare elements. S. Chand & Co, IV Edn (1986).
- 11. K.M.Mackay and R.A. Mackay, Introduction to Modern Inorganic Chemistry, 4th Edn, Prentice Hall, New Jersy 1989.
- 12. M. C. Day, J. Selbin and H. H. Sisler, Theoretical Inorganic Chemistry; Literary Licensing (LLC), Montana, 2012.
- 13. F. A. Cotton and G. Wilkinson, C. A. Murillo and M. Bochmann, Advanced Inorganic Chemistry; 6th Ed., A Wiley Interscience Publications, John Wiley and Sons, USA, 1999
- 14. J. E. Huheey, Inorganic Chemistry; 4th Ed., Harper and Row publisher, Singapore, 2006



I YEAR – I SEMESTER COURSE CODE: 7MCH1C3

CORE COURSE-III-PHYSICAL CHEMISTRY-I

Objectives:

- ✓ To enable the learners to understand the significance of electrochemistry
- ✓ To know the details of phase rule, thermodynamics and surface chemistry.

Unit I: Electrolytic conductance and Electro kinetics

[15 Hrs]

Theory of electrolytic conductance – ionic activity and activity coefficient – Ionic strength – Debye – Huckel theory – Limiting Law – Ionic association – Molar conductivity – Debye – Huckel – Onsager equation – Applications of conductivity measurement – Electrode potential – Helmholtz electrical double layer – Standard electrode potentials – Nernst equation – Applications of Nernst equation – Electrochemical cells and their types – Applications of cell EMF measurements (G, S and H calculations). Calculation of equilibrium constants and solubility products – Over voltage – Hydrogen overvoltage – Butler -Volmer equation, Tafel equation.

Unit II: Classical Thermodynamics

[15 Hrs]

Terminology in thermodynanics – I-law of Thermodynamics – limitations – Need for Second law of thermodynamics – Second law of thermodynamics Statements – concept of entropy – Gibbs and Helmhotz free energy – Spontaneity – Gibbs-Helmholtz equation – Van't Hoff Isotherm – Partial molar quantities, partial molar volume – chemical potential, Gibbs -Duhem equation – Experimental determinations of fugacity of real gases and its determination – activity and activity co-efficient – determination.

Unit III: Chemical and Phase Equilibria

[15 Hrs]

Chemical Equilibria: Spontaneous reaction – Free energy change for Spontaneous reaction – Significance – Law of mass action, Equilibrium Constant – Van't Hoff equations – Types of equilibrium – Le-Chatelier's Principle – Factors affecting chemical equilibrium.

Phase Equilibria: Gibbs Phase rule – Derivations of Gibb's Phase rule – Two component systems (KI-H₂O system, FeCl₃-H₂O system, Zinc-Magnesium System, Sodium sulphate and water system)

Unit IV: Statistical Thermodynamics

[15 Hrs]

Aims of statistical thermodynamics – thermodynamic probability – probability theorem – definitions of state of a system – ensembles (micro, macro and grand canonical) – Boltzmann distribution law and its derivations – Boltzmann-Planck equation – Partition functions – thermodynamic properties from partition functions – partition function and equilibrium constant – Quantum statistics – Fermi-Dirac and Bose-Einstein statistics – population inversion.

Unit V: Colloids and Surface Chemistry

[15 Hrs]

Colloids: Classification of Colloids – Sols, Lyophilic and lyophobic sols, properties of sols, coagulation. Electrical properties of colloids – Charge on colloidal particles – Electrical double layer – Zeta potential – Electro kinetic properties – Electrophoresis – Electro osmosis.

Surface Chemistry: Introduction – adsorption of gases on solids – physisorption and chemisorptions – adsorption isotherms – Freundlich – Langmuir – BET – Temkin adsorption isotherms – adsorption on liquid surface – surface tension – Gibbs adsorption isotherm – surface area determination by electro-osmosis and electrophoresis.

Books for Reference:

- 1. J.Rajaram and J.C.Kuriakose, Thermodynamics (III Edn.) shoban Lai Nagin, Chand & Co., New Delhi (1999).
- 2. D.Attwood and A.T.Florence, surfactant systems Their chemistry, Pharmacy and Biology, Chapmann and Hall, New-York (1983).
- 3. S.Glasstone, Thermodynamics for chemists, East West Press private Ltd., New Delhi.
- 4. Gurdeep Raj, Advance Physical chemistry (25th Edn.,) Goel Publishing Co., Publishing Co., (2001).
- 5. D.A.Mc Quarrie and J.D.Simon, Physical chemistry. A molecular Approach, Viva Books (p) Ltd., New Delhi (1998).
- 6. P.W.Atkins, physical chemistry. VI, Edn., ELPS and Oxford University Press (1996).
- 7. A.W.Adamson, Physical Chemistry of Surfaces, 5th Edn., John Wiley & Sons, New York, (1990).
- 8. L.Antropov. Theoretical electrochemistry MIR Publication Moscow 1972.
- 9. A.W.Adamson, physical chemistry of surfaces, 5th Edn., John Wiley & sons, New York (1990).
- 10. B.R.Puri, L.R.Sharma and M.S.Pathania, Principles of Physical chemistry (Millennium Edn,) Vishal Publishing Co., (2003).
- 11. D.N.Bajpai, Advanced physical chemistry, S.Chand & Company Ltd, New Delhi (1998).
- 12. J.O.M. Bockris and A.K.N. Reddy, Electrochemistry, Vols. 1 and 2, Plenum, New York 1977.
- 13. C.M.A.Brett and A.M.O.Brett, Electrochemistry, Principles, Methods and application, OUP, Oxford (1993)



I YEAR – I SEMESTER COURSE CODE: 7MCH1P1

CORE COURSE-IV-INORGANIC PRACTICAL-I

Objectives:

- Zero enable the learners to apply the principle in the semi-micro analysis of an inorganic salt mixture.
- - 1. Semi micro qualitative analysis: Analysis of mixtures containing one familiar and one less familiar cations from the following W, Pb, Se, Te, Mo, Cu, Cd, As, Sb, Ce, Th, Zr, Ti, V, Cr, Mn, U, Ni, Co, Zn, Ca, Ba, Sr, Li, Mr (insoluble and interfering anion may be avoided).
 - 2. Estimation of one metal ion in the presence of another by EDTA.
 - 3. Inorganic preparations: preparation of at least 5 inorganic complexes.

Books for Reference:

- 1. J. Bassett *et al*, Text Book of Quantitative Chemical Analysis", 5th Edition, ELBS, Longmann, U.K., 1989.
- 2. V.V. Ramanujam, "Inorganic Semimicro Qualitative Analysis", The National Publishing Co, Chennai 1974.

I YEAR – I SEMESTER COURSE CODE: 7MCH1E1

ELECTIVE COURSE-I (A)-APPLIED CHEMISTRY

Objectives:

- Z To enable the learners to understand the water, Raw materials, Petroleum and Fuels.

Unit I: Water [15 Hrs]

Methods of Treatment of water for domestic supply - Sedimentation, Coagulation, Filtration, Sterilization, Break point chlorination. Hardness - Different types of hardness - Determination of Hardness of water: Demineralization of water by Ion exchange process, Zeolite process and Reverse osmosis process. Boiler Troubles: Carry Over, Priming, Foaming, Scale, Sludge and Caustic Embrittlement. Internal treatment of water - Carbonate conditioning, Phosphate conditioning, Colloidal conditioning and Calgon conditioning.

Unit II: Raw materials, Petroleum and Fuels

[15 Hrs]

Industrial Raw materials – Characteristics of raw materials and their resources – methods of raw material concentrations – integral utilization of raw materials - Energy for chemical industry – Fuels – classification of fuels – Characteristic properties of solid, liquid and gaseous fuels - Petroleum, cracking, Synthetic petrol, Refining of gasoline, Reforming, knocking properties - Octane Rating of petrol, Cetane Rating of Diesel - Composition and uses of coal gas, water gas, producer gas, oil gas, LPG and gobar gas.

Unit III: Cement, Glass and Fertilizers

[15 Hrs]

Manufacture of cement, Dry and Wet process, important process parameters for manufacturing a good cement clinker. Setting Mechanism of Cement – Different types of cement – Special Cement – White Cement.

Glass: Composition of Glass – Raw materials for Manufacture of Glass – Manufacturing of Glass – Composition and Uses of Optical glass, colored glasses, lead glass and neutron absorbing glass.

Fertilizers: Definition of Fertilizer - Fertilizer industries in India, Manufacture of ammonium salts, urea, Di-ammonium phosphate – superphosphate and triple superphosphate.

Unit IV: Sugar and Agro Chemicals

[15 Hrs]

Sugar: Cane sugar manufacture, recovery of sugar from molasses, sugar estimation, sugar industries in India.

Agrochemical industries: Important categories of insecticides, fungicides, herbicides. Mode of action and synthesis of common pesticides like Gammexane, DDT, alathrin, Parathion, Malathion, Baygon, DDVP, Warfarin.

Unit V: Lubricants & Protective Coatings

[15 Hrs]

Lubricants: Functions of lubricant, Mechanism of lubrication, classicification of lubricants – Lubricating oil – Greases - Properties of lubricating oil and Greases – Solid lubricants (Graphite and Molybdenum)- Fluid or Hydrodynamic Lubrication, Thin film or Boundary lubrication & Extreme pressure lubrication.

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.

Books for Reference:

- 1. B.K Sharma Industrial chemistry Goel publishing house, 2006.
- 2. A text book of Engineering Chemistry by S. S. Dara, S. Chand & Co. New Delhi 2010.
- 3. Engineering Chemistry by Jain & Jain, Dhanpat Rai _Publishing Compony, New Delhi, 2009.

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I YEAR – I SEMESTER COURSE CODE: 7MCH1E2

ELECTIVE COURSE-I (B)-POLYMER CHEMISTRY

Objectives:

Zero enable the learners to understand the chemistry of polymers, kinetic mechanism and their degradation.

Unit I: Classification of Polymers and Chemistry of Polymerisation [15 Hrs]

Classification of Polymers, linear polymers, non-linear or branched polymers, cross – linked polymers, homo chain, hetero chain, homopolymers co-polymers, block polymers and graft polymers. Degree of polymerization: Types of polymerization – mechanism of Addition polymerisation – (Free radical, ionic and co-ordination mechanism) – Rubber and Vulcanisation of Rubber.

Unit II: Individual Polymers

[15 Hrs]

Individual Polymers: Preparation, properties and applications of polystyrene, polyacrylonitrile, polymethylmethacrylate, Polytetrafluoroethylene, polybutadienes and polychloroprene, polyesters, polycarbonates, polyimides, polyamides (Kevlar), polyurethanes, polyethylene, phenol – formaldehyde, urea – formaldehyde, melamine – formaldehyde and epoxy resins.

Unit III: Properties of Polymers

[15 Hrs]

Intrinsic properties – processing properties – basic idea of isomerism of polymers – configuration of polymer chain – geometrical structure – syndiotatic, isotatic and atatic polymers.

Glass transition temperature: Definition – factors affecting glass transition temperature – relationships between glass transition temperature and (a) molecular weight, (b) melting point and (c) plasticizer.

Molecular weight and size of polymers: Number average, weight average, sedimentation and viscosity average molecular weights – molecular weights and degree of polymerization – poly-dispersity – molecular weight distribution in polymers – size of polymer molecules – kinetics of polymerization.

Unit IV: Polymerisation Techniques and Degradation of Polymers [15 Hrs]

Polymerisation Techniques: Bulk, solution, suspension, emulsion, melt condensation and interfacial polycondensation polymerizations, Degradation: Types of degradation – thermal, mechanical, ultrasonic and photo degradation – photo stabilizers – oxidative degradation – antioxidants – hydrolytic degradation.

Unit V: Polymer Processing

[15 Hrs]

Compounding of plastics, Rubber and fibres – (plasticizers, colorants, flame retardants) - Polymer processing - Compression, blow and injection mouldings – film extrusion and calendaring – die casting and rotational casting – thermo foaming – reinforcing. Biopolymers – Biomedical polymers – Contact lens, Dental polymers, Artificial Heart, Kidney, Skin and Blood cells.

Books for Reference:

- 1. V.R.Gowarikar, N.V. Viswanathan and Jayadev Sreedher, "Polymer Science", Wiley Eastern Ltd., New Delhi, 2001.
- 2. B.K.Sharma, "Polymer Chemistry", Goel Pub., House, Meerut, 2009.
- 3. F.W.Billmeyer, "Text Book of Polymer Science", 3rd edn., John Wiley and sons, New York, 2004.
- 4. P.Bahadur, N.V.Sastry, Principles of Polymer Science, II nd Edn., Narosa Pub. House Pvt. Ltd., New Delhi, 2005.
- 5. G.S.Mistra, Introductory Polymer Chemistry, New Age International Pub., New Delhi, 2005.

I YEAR – II SEMESTER COURSE CODE: 7MCH2C1

CORE COURSE-V-ORGANIC CHEMISTRY-II

Objectives:

- To study the detailed aspects of conformational analysis, analytical techniques like ¹H NMR and ¹³CNMR.
- > To know about various oxidation and reduction reactions in detail and their reagents.
- > To study about detailed chemistry of steroids.

Unit I: Conformational Analysis

[15 Hrs]

Configuration and Conformation – Conformations of Ethane and n-Butane – Conformational Analysis – Stereoelectronic and Steric factors – Conformation of Simple Acyclic Compounds – Conformation of Monosubstituted and Disubstituted Cyclohexanes – Correlation of the Conformation of Acyclic and Cyclic Systems with their Physical and Chemical Properties – Conformational Free Energy Difference – Determination of Conformational Free Energy difference – Quantitative Treatment of Mobile System – Eliel - Ro Equation

Unit II: Spectroscopy

[15Hrs]

UV Spectroscopy – Principle – Absorption Spectra of Conjugated Dienes, α , β -Unsaturated Carbonyl Compounds – Woodward Rules – Calculating of λ max. IR Spectroscopy – Molecular Vibrations – Vibrational Frequency – Factors Influencing

IR Spectroscopy – Molecular Vibrations – Vibrational Frequency – Factors Influencing Group Frequencies – Quantitative Studies.

Mass Spectroscopy – Principle – Type of Ions – Base Peak – Parent Ion, Metastable Ion and Isotopic Ions – Fragmentation – General Rules – Pattern of Fragmentation for Various classes of Compounds – Mc Lafferety Rearrangement – Retro Diels – Alder Reaction.

Unit III: NMR Spectroscopy

[15 Hrs]

¹H – NMR Origin of NMR Spectra – Chemical Shift. Spin-Spin Coupling – Coupling Constant – First Order and Second Order Spin-Spin Splitting – Influence of Stereo chemical Factors on Chemical Shift of Protons – Simplification of Complex Spectra – Spin Decoupling – Double Resonance – Shift Reagents, CIDNP.

 13 C - NMR Spectroscopy - Basic Principle of FT Technique - Relaxation Time - Assignment of the Signals - Off-Resonance Decoupling - 2D NMR. Structural Problems based on all the above Techniques.

Unit IV: Oxidation and Reduction – Reagents in Organic Synthesis [15 Hrs]

a) **Oxidation:** Mechanism, Applications and Stereo Chemical Aspects of the Oxidations using Chromic Acid, Selenium Dioxide, Osmium Tetroxide, N – Bromo Succinimide, Oppenauer Oxidation.

- b) **Reduction:** Catalytic Reduction (homogeneous and heterogeneous) Reductions using LiA1H₄, DIBAL and Sodium Borohydride Birch Reduction Meerwein-Pondorf- Verley Reduction Hydroboration.
- c) **Reagents in Organic Synthesis:** Lithium Dimethyl Cuprate, Lithium Diisopropylamide (LDA), Dicyclohexyl Carbodiimide, 1,3-Dithiane (umpolung), Woodward and Prevost Hydroxylation, DDQ, Phase Transfer Catalyst (quaternary ammonium salt, crown ethers).

Unit V: Steroids [15 Hrs]

Classification – conformational aspects of A/B Cis and A/B trans steroids – complete chemistry and stereochemistry of cholesterol (includes bile acid) and ergosterol.

Vitamin D_2 – Male sex hormones – Androsterone and testosterone – female sex hormones – Oestrone and progestrone – A basic idea about adrenocortical hormones – Cortisone (synthesis only).

Books for Reference:

- 1. Eliel E.L., Stereochemistry of Carbon Compounds McGraw-Hill, New Delhi, 1962.
- 2. Eliel E.L., Stereochemistry of Carbon Compounds, Wiley Eastern, New York, 1994.
- 3. Kalsi P.S., Stereochemistry, Conformation and Mechanism, Wiley Eastern Ltd., 7th Edition, New Delhi, 2009.
- 4. Mislow K., Introduction to Stereochemistry, Benjamin, London, 1966.
- 5. Nasipuri D., Stereochemistry of Organic Compounds, Principles and Application, Wiley Eastern Ltd., 2nd Edition, New Delhi, 1994
- 6. Dyer J.R., Application of Absorption Spectroscopy, 2nd Edition, Prentice–Hall, Hampshire, 1965.
- 7. Howe I., Williams D.H. and Bowen R.D., Mass Spectrometry, Principles and Applications McGraw Hill, 2nd Edition, New Delhi, 1981.
- 8. Kemp, Organic Spectroscopy, ELBS, 3rd Edition, Hampshire, UK, 1987.
- 9. Silverstein B.M., Bassler G.C., and Morrill T.C., Spectrometric Identification of Organic Compounds. Wiley, 8th Editionn., New York, 2014.
- 10. Carruthers W., Some Modern Methods of Organic Synthesis, Cambridge University Press, 4th Edition., London, 2004.
- 11. House H.O., Modern Synthetic Reactions, Benjamin W.A., Inc. California, 2nd Edition, California, 1972.
- 12. Norman R.O.C., Organic Synthesis, 3rd Edition, London, 1993.
- 13. Pinc S.H., Hendrickson J.B., Cram D.J., and Hammond G.S, Organic Chemistry, McGraw–Hill Kogakusha Ltd., Tokyo 4th Edition, 1980.
- 14. Finar I.L., Organic Chemistry, Vol. 11, ELBS. England, 1975.

I YEAR – II SEMESTER COURSE CODE: 7MCH2C2

CORE COURSE-VI-INORGANIC CHEMISTRY-II

Objectives:

- Z To have an insight into study of coordination compounds, and their reactions.
- Z To know the details of bioinorganic chemistry and nuclear chemistry.

Unit I: Coordination compounds

[15hrs]

Nomenclature of coordination complexes – labile and inert complexes – stability constants of complexes – stepwise and overall stability constant – their determination-Jobs'continuous variation method and spectrophotometric method – factors affecting the stability constants. VBT – explanation with examples-draw backs of VBT.

CFT- Influence of ligands on crystal field splitting – octahedral and tetrahedral splitting of "d" orbitals, CFSE, CFSE Calculation in terms of D_q . Spectrochemical series and magnetic properties.

Unit II: Reaction Mechanism of Coordination compounds [15hrs]

Substitution reactions – square planar substitution reactions – Factors affecting reactivity of square planar complexes –Trans effect – theories of Trans effect – substitution reactions in octahedral complexes. (SN_1,SN_2,SN_iCB) – reactions of coordinated ligands – acid hydrolysis – anation reactions and base hydrolysis.

Mechanism of electron transfer reactions – Outer sphere, inner sphere electron transfer reactions. Synthesis of coordination compounds using electron transfer and substitution reaction – applications of coordination compounds.

Unit III: Bio-Inorganic Chemistry

[15hrs]

Porphyrin ring system – metalloporphyrins – hemoglobin and myoglobin structures and work functions – synthetic oxygen carries – cytochromes and ferridoxins – structure and work functions in respiration – chlorophyll – structure – photosynthetic sequence – iron sulphur proteins [non - heme iron protein]. Copper containing proteins – classification – blue copper proteins – nitrogen fixation (in-vivo and in-vitro nitrogen fixation).

Unit IV: Reactions and Catalysis using Organometallic compounds [15 hrs]

Organometallic reactions – ligand association and dissociation – oxidative addition and reductive elimination – insertion reactions. Catalytic mechanism in the following reactions – hydrogenation of olefins (Willkinson catalyst) – Tolman catalytic loops hydroformylation (Oxoprocess) – acetic acid from methanol– oxidation of alkenes to aldehydes and Ketones (Wacker process) – synthesis gas and their applications using organo metallic compounds as catalyst – olefin polymerization (Ziegler-Natta), Cyclo oligomerisation of acetylenes (Reppe's or Wilke's catalysts).

Unit V: Nuclear chemistry

[15 hrs]

Radioactive decay and equilibrium- different types of nuclear reaction – spallation – fission and fusion – theories of fission – fissile and fertile isotopes characteristics of Nuclear fission and fusion – Nuclear fusion – stellar energy.

Nuclear forces: Liquid drop model and shell model. Nuclear reactors – classification of nuclear reactors – breeder reactor. Applications of radioactive isotopes in chemical investigations, age determination, medicinal and agricultural field.

Books for Reference:

- 1. W.E Addison, Structural Principles of Inorganic Chemistry, Wiley 1961.
- 2. A.F. Wells, Structural Inorganic Chemistry, 4th edition, Oxford. New York 1984.
- 3. F.A. Cotton and G.Wilkinson, Advanced Inorganic Chemistry 6th Edn. John Wiley and Sons, Singapore 1999.
- 4. K.F. Purcell and J.C. Koltz, An Introduction to Inorganic Chemistry, W.B. Saunders Company, Philadelpha 1980.
- 5. J.E.Huheey, E.A.Keiter and R.L.Keiter, Inorganic Chemistry Principles of structure and reactivity, 4th Edition, Pearson Education, 2002.
- 6. S. Glasstone, Source Book for Atomic Energy, 3rd edn., Van Nostrand Reinhold Company, New York, 2014.
- 7. S.F.A, Kettle, Coordination Chemistry Ari Approach, Spectrum Academic publishers Oxford, 1996.
- 8. I. Bertini et al Bioinorganic Chemistry, Viva Books private Ltd, Chennai, 1998.
- 9. G.S.Manku, Inorganic Chemistry, TMH Co., 1984.
- 10. C.N.R.Rao and J.R.Ferraro, Spectroscopy in Inorganic Chemistry, Vol. I and Vol. II Academic Press, 1971.
- 11. H.A.O. Hill and P.Day, Physical methods in advanced Inorganic Chemistry, John Wiley, 1986.
- 12. R. C. Mehrotra and A. Singh, Organometallic Chemistry; 2nd Ed., New Age International Ltd. New Delhi, 2014.
- 13. A. W. Parkins and R. C. Poller, An Introduction to Organometallic Chemistry; 1987, Oxford University Press, Chennai.
- 14. H.J. Arnikar, IV Edn., Essentials of Nuclear Chemistry, New Age international (P) Ltd., New Delhi. 2005.

I YEAR – II SEMESTER COURSE CODE: 7MCH2C3

CORE COURSE-VII-PHYSICAL CHEMISTRY-II

Objectives:

- Z To enable the learners to understand the principles of chemical kinetics.

Unit I: Chemical Kinetics

[15 Hrs]

Basic concept – Rate law – Rate equation – order – Molecularity – Chain reactions – general characteristics – Steady state approximations – study of kinetics of chain reactions like H_2 - Br_2 reaction – decomposition of acetaldehyde and N_2O_5 – Explosive reactions -Study of H_2 - O_2 explosive reactions. Arrhenius theory – Collision theory – Absolute reaction rate theory –Unimolecular reaction rate theories – the simple Lindemann treatment – Hishelwood's theory – Rice, Ramsperger and Kassel (RRK) theory – Advanced unimolecular theory – Marcus theory or Rice, Ramsperger, Kassel and Marcus (RRKM) theory.

Unit II: Rotational and Infrared Spectroscopy

[15 Hrs]

Electromagnetic spectrum – Types of molecular energies – Einstein's coefficient — Rotational spectra of rigid diatomic molecules – isotope effect in rotational spectra – Microwave spectrometer – Information derived from rotational spectra.

Infrared spectroscopy – vibrational energy of diatomic molecule – infrared selection rules – diatomic vibrating rotator – concept of group frequencies – coupling interaction – Fermi resonance – Fourier transform infrared spectroscopy.

Unit III: Raman and Electronic Spectroscopy

[15 Hrs]

Raman spectroscopy – Theories of Raman scattering – Rotational Raman spectra – vibrational Raman spectra – Mutual exclusion principle – Laser Raman spectra.

Electronic spectra of diatomic and polyatomic molecules intensity of vibrational electronic spectra – Franck Condon principle – the Fortrat parabola – Dissociation and predissociation spectra.

Photoelectron spectroscopy – basic principles, spectrum, X-ray PES, (ESCA) – vibrational structure – koopman's theorem – PES of argon, oxygen and nitrogen.

Unit IV: NQR, NMR & ESR Spectroscopy

[15 Hrs]

NQR – Principles and applications – quadrupole moment and electrical field, nuclear quadrupole resonance, nuclear quadrupole coupling in atoms and molecules – identification of ionic character and hybridization.

NMR: Principles of NMR – Relaxation Process – Mechanism of Relaxation process – Chemical shift – Representation of spectrum – Complex spectra – Decoupling – NOE – Chemical Shift reagents.

ESR: Principles of ESR – Isotropy and Anisotropy – Hyperfine structure – ESR spectra of free radicals in solution (Hydrogen atom, Methyl, phenyl and Naphthyl radical) – zerofield splitting in ESR and Krammer's degeneracy.

Unit V: Group Theory

[15 Hrs]

Molecular symmetry elements and symmetry operations – transformation matrices – Group – definition and properties of a group – symmetry point groups – representation of a group –reducible and irreducible representations – Great orthogonality theorem – characters – construction of a character tables – C_2V and C_3V . Projection operators – direct product representation – Prediction of symmetries of atomic orbital – symmetries of tensor like properties ($\alpha \& \beta$) – Application to predict the selection rules for IR / Raman activity of normal modes of H_2O and NH_3 . Prediction of orbitals and hybridization for the molecules BF_3 and CH_4 .

Books for Reference:

- 1. K.J.laidler, Chemical Kinetics, 3rd Edn., Harper International Edn., London (1987).
- 2. F.A.Cotton, chemical applications of Group theory, 3^{rrJ} Edn. John Wiley & Sons, New York (1999)
- 3. K.V.Raman, Group Theory and its Applications to chemistry, Tata McGraw-Hill (1990).
- 4. Symmetry and molecular spectroscopy K. Veera Reddy.
- 5. C.N.Banwell and E.M.Mc Cash, Molecular Spectroscopy, Tata McGraw Hill, 4th Edn., (1995).
- 6. G.H.Barrow., Introduction to Molecular Spectroscopy, McGraw Hill
- 7. R.Chang, Basic Principles of Spectroscopy, McGraw Hill London (1976).
- 8. A Simple approach to group Theory in chemistry S.Swarnalakshmi, T.Saroja, R.M Ezhilarasi.
- 9. V.Ramakrishnan and Gopinath, Group Theory in chemistry, 2nd edn.. vishal publications, 1991.
- 10. W.Kemp, NMR in Chemistry, MacMillan Ltd, 1986.
- 11. G.W.King, Spectroscopy and Molecular structure, Holt, Rienehart and Winston, 1964.
- 12. B.F.Straughan and S.Walker (eds.), Spectroscopy, vol. 1, 2 and 3, Chapman & Hall Londan(1976).
- 13. P.W. Atkins, Physical Chemistry, 6th edn., Oxford University Press, Tokyo(1998).



I YEAR – II SEMESTER COURSE CODE: 7MCH2P1

CORE COURSE-VIII-ORGANIC PRACTICAL-I

Objectives:

- Z To enable the learners to understand the principles organic qualitative and quantitative analysis.
- Z To train the students to become a skill person in organic preparations.

1. Qualitative Analysis

Separation and Analysis of two component mixtures. Identification of the components and preparation of solid derivative.

2. Quantitative Analysis

- a. Estimation of glucose by Lane and Eynon method and Bertrand method.
- b. Estimation of Glycine.
- c. Estimation of methyl ketone

3. Organic Preparations

Two stage process. (At least any 5 preparations)

Books for Reference:

- 1. Vogel's Practical Organic Chemistry.
- 2. Laboratory manual of organic chemistry B.B. Dey and M.V. Sitaraman.

I YEAR – II SEMESTER COURSE CODE: 7MCH2E1

ELECTIVE COURSE II (A) – ENVIRONMENTAL CHEMISTRY

Objective

To understand the Pollutant, pollution, prevention of pollution and analysis.

Unit I: Atmosphere & Air Pollution

[15 Hrs]

Concept & scope of Environmental chemistry; Environmental segments; Environmental Pollution; Classification of pollutants; Bio-geological cycles in the environment: Hydrological cycle, C, N, O, S and P cycles in the environment; Bio-distribution of elements; Structure and Composition of Atmosphere; Particles, Ions & Radicals in the atmosphere; Major sources of Air Pollutants. Pollution by C, CO, NO_X, SO_X, HC, Acid Rain, Smog, Particulates; Green House effect/Global Warming, Ozone Layer depletion; Effects & Control of Air Pollutants

Unit II: Hydrosphere and Water Pollution

[15 Hrs]

Aquatic environment, Chemical composition of water bodies; Lakes, Streams, Rivers. Various water resources and their characteristics; water pollution – source and classification; organic inorganic and radioactive pollutants; sampling and analysis of water pollutants; water quality parameters and standards; determination of water quality parameters. Fluorosis and defluoridation; water treatment processes and preservation. Some case studies of water pollution.

Unit III: Lithosphere and Soil Pollution

[15 Hrs]

Introduction: Soil formation, composition & classification; Acid-Base and Ion-exchange reactions in Soil; Macro-and Micronutrients, Soil Profile; Soil fertility and Productivity, Soil erosion, Soil Analysis (Moisture, Nitrogen & pH).

Soil Pollution: Sources & Classification. Chemical composition; micro and macro nutrients in soil; pollution by fertilizers, persticides, plastics and heavy metal compounds. Plant as indication of soil pollution; treatment and abatement procedures for soil pollution.

Unit IV: Industrial Pollution, Radiation pollution & Environmental toxicology [15 Hrs]

Introduction-causes of industrial pollution-thermal power plants-nuclear power reactors-fertilizers and chemical industry-pulp and paper industries-agro based industries-cement industry.

Classification & effects of radiation, effects of ionizing radiation on man, Effects of non ionizing radiation on life, radioactivity and Nuclear fallout, protection and control from radiation.

Toxic chemicals in the environment-biochemical effects of arsenic, cadmium, lead, mercury and cyanide-bio-ware agents. Chemical solutions to environmental problems biodegradability, principles of decomposition better industrial processes, Bhopal gas tragedy, Chernobyl, three mile island, sewozo and minamata disasters.

Unit V: Disaster Management

[15 Hrs]

Types of Disasters; Disaster prevention; Disaster preparedness; Disaster Relief; Recovery; Cyclones: Types of cyclones; How cyclones are formed?; What is an Earthquake?:

Why do earthquakes happen?; Size and Frequency; Human Induced Seismic Activity; Impact of earthquakes; Tsunami; Nuclear accidents and Holocaust; Case Studies of Nuclear accidents.

Books for Reference:

- 1. Environmental Chemistry, A.K. De, Wiley Eastern Ltd, 3 rd edn., 1994
- 2. Environmental Chemistry, B.K. Sharma, Goel Publishers, 2001.
- 3. Environmental Chemistry, M.S. Sethi, Sri Sai Printographers, 1994.
- 4. Text book of Environmental Chemistry, C.D. Tyagi and M. Mehra, Anmol Publishers, 1996.
- 5. Fundamentals of Environmental Pollution, K. Kannan, S. Chand and Co., 1997.
- 6. Environmental Chemistry: Edited by J. O'M. Bockris, Plenum Press.
- 7. Environmental Chemistry: S.E. Manahen, Lewis Publications.
- 8. Environmental Chemistry: H. Kaur, Pragati Prakashan.
- 9. Shweta Sharma and Pooja Sharma, Environmental Chemistry: Narosa Publishing House Pvt.Ltd.,New Delhi, 2014.
- 10.Physico-chemical Examination of Water, Sewage & Industrial Effluents: K. Manivasakam.

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I YEAR – II SEMESTER COURSE CODE: 7MCH2E2

ELECTIVE COURSE-II (B)-COMPUTER IN CHEMISTRY

Objectives

- Z To study the basic concepts of computers and applications in the chemistry.
- ✓ To know about basic concepts of internet and cheminformatics.

Unit I: Introduction to computers and computing

[15 Hrs]

Significant developments in the history of computers-computer generations—Components of a computer-block diagram-CPU, ALU, control units, memory unit, Memory—classification of memory devices, Main memory—semiconductor memory devices (RAM, ROM—Secondary memory devices—magnetic disks (hard and floppy)—Peripheral devices—Input devices—keyboard keys and their uses-mouse; Output devices—VDU-printer and its classification; Hardware and software. Introduction to UNIX and WINDOWS, data processing, principles of programming, algorithms and flow-charts.

Unit II: Applications of C Language in Chemistry-I

[15 Hrs]

Explanation of the formulae, equations and programs to solve the following problems in chemistry:

- 1. Calculation of Molecular weight of Organic Compounds.
- 2. Calculation of pH.
- 3. Determination on First Order rate constant for the given reaction
- 4. Evaluation of lattice energy using
 - i) Born- Haber Cycle
 - ii). Born -Lande equation
- 5. Computing ionic radii- Lande's method and Paulings method
- 6. Calculation of Normality, Molarity and Molality of a given solution
- 7. Converting Kelvin to Celsius temperature and vice versa.
- 8. Determination of enthalpy of a given solution
- 9. Evaluation of Cell constant
- 10. Calculation of energy of Hydrogen atom spectral lines.

Unit III: Applications of C Language in Chemistry-II

[15 Hrs]

Explanation of the formulae, equations and programs to solve the following problems in chemistry:

Organic Chemistry:

1. Use of Recursive functions to calculate the number of □ Resonance structures for an organic conjugated system using

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res - str = n! / ((n/2)! * ((n/2) + 1)!)
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2. Empirical formula of Hydrocarbons and other Organic compounds.

Inorganic Chemistry:

- 1. Array manipulation to balance the chemical equations.
- 2. Half life and average life periods of radioactive nuclei.
- 3. Binding energy of nucleus.
- 4. Program to get output as First ten elements of Periodic Table with their Name, Symbol, Atomic number and Atomic Weight.

Physical chemistry:

- 1. Calculation of RMS, average and MPV of gases.
- 2. Solving Quadratic equation to evaluate the Equilibrium constant for the reaction

$\mathbf{H}_2 + \mathbf{I}_2 \quad \leftrightarrow \ \mathbf{2HI}$

- 3. Illustrate use of Loop to calculate the NMR frequency for a nucleus with Spin ½
- 4. Mean activity coefficient of an Electrolyte (KCl)

Unit IV: Internet and E-mail

[15 Hrs]

INTERNET: Introduction- History- Importance of the Internet-Internet Access- Dial-Up connection, Direct connection and equipments-Internet protocol(TCP/IP,FTP,HTTP, TELNET and WAP)-Internet addressing-Domain Name-Mail address-Uniform Resource Locator(URL)-Web Browsing- Searching the Web- Search Engines(Yahoo, Google)-Intranet Searching and utilizing Popular websites in Chemistry. On line literature survey- accessing of e-journals. Preparing articles for e-publications. Online structure drawing-Collection of spectral data using databases.

ELECTRONIC MAIL: Introduction-Working of E-Mail-Word processor for E-Mail- Mailing Basics—Composing and sending of an E-Mail-Address Book—Signature-File Attachments-Customizing your Mail program—Advantages and Disadvantages of E-Mail-Tips for effective E-Mail use-Smile keys.

Unit V: Cheminformatics

[15 Hrs]

Introduction-definition, scope and use of cheminformatics, chemical database and chemical resources, search methods in cheminformatics; applications in drug discovery-evolution and process, major goals and strategies of drug discovery-development of the drug: the five classic steps, the current roles and uses of the computer in drug design—software using in drug design—preparing chemical mode through chemsketch and chemdraw softwares.

Books for Reference:

- 1. K. V. Raman, Computers in Chemistry, Tata McGraw-Hill Publishing Company Ltd., New Delhi, 3rd Edn., 1993.
- 2. K. Arora, Computer Applications in Chemistry, Anmol Publications Pvt. Ltd. 2004.
- 3. R. Kumari, Computers and their Applications to Chemistry, Narosa Publishing House Pvt. Ltd. Second Edition 2005.
- 4. David Jung, Pierre Boutqukin, John D. Conley III, Loren Eidahl, Visual Basic 6 Super Bible, First Indian Edition, Techmedia, New Delhi, 1999.
- 5. Gary Cornell, Visual Basic 6. Tata-McGraw Hill, New Delhi, 1998.
- 6. E. Balagurusamy, Programming in ANSI C, Tata McGraw- Hill Publishing Company Ltd., New Delhi, 3rd Edn., 10th Reprint, 2005.
- 7. Yeshavant Kanitkar, Let Us C, BPB Publications, New Delhi, 3rd Edn., 1999.
- 8. Brian W. Kernighan & Dennis M. Ritchie, The C Programming Language, Prentice Hall of India Private Limited, New Delhi, 2nd Edn., 2001.
- 9. Byron S. Gottfried, Programming with C, Tata McGraw-Hill Publishing Company Ltd., New Delhi, 2nd Edn., 2001.
- 10.R. Rajaram, C Programming Made Easy, Scitech Publications, Chennai, 1999.\

II YEAR – III SEMESTER COURSE CODE: 7MCH3C1

CORE COURSE-IX-ORGANIC CHEMISTRY-III

Objectives:

- Z To have a knowledge of Molecular rearrangement and addition reactions.

Unit I: Reactions and Rearrangements

[15 Hrs]

Mechanism of the following rearrangements: Wagner-Meerwin, Dienone-phenol rearrangement, Demjanov, Curtius, Wolff, Baeyer -Villiger, Stevens, Favorski, Cope, Fries and Di-pi methane rearrangement. Mechanism of sommelet reaction – vilsmeir haak reaction – Arndt-Eistert reaction.

Unit II: Addition to multiple bond

[15 Hrs]

Electrophilic, Nucleophilic and free radical additions – Addition to Conjugated Systems – Orientation of the addendum – Sharpless asymmetric epoxidation, Addition to α, β – unsaturated Carbonyl groups.

Michael addition – Addition of Grignard reagent to α , β – unsaturated carbonyl groups. Diels- Alder reaction – Addition of Carbenes and Carbenoids to double and triple bonds.

Addition to Carbonyl Group: Mechanism of Mannich reaction, Claisen ester condensation, Darzen's reaction, Reformatsky reaction, wittig reaction and Shapiro reaction.

Unit III: Terpenoids

[15 Hrs]

Terpenoids: Classification of terpenoids, structure, and synthesis of α -pinene, Camphor, Zingiberene, Cadinene and abietic acid – Biosynthesis of terpenoids.

Unit IV: Synthetic Methods

[15 Hrs]

Planning a synthesis – relay approach and convergent approach to total synthesis – Retro synthetic analysis of simple organic compounds – Functional group interconversions – use of activation and blocking groups in synthesis – Homogeneous hydrogenation – Umpolung synthesis – Robinson annelation – A schematic analysis of total synthesis of the following compounds: 2, 4 – dimethyl-2-hydroxypentanoic acid, Trans-9-methyl-1-decalone.

Unit V: Organic Photochemistry

[15 Hrs]

Thermal Vs Photochemical reactions – Allowed and forbidden transitions – Fluorescence – Internal conversion – Intersystem crossing – Jablonski diagram.

Photochemical reactions of Ketones – photosensitization – Norrish type I and Norrish type –II reactions – Paterno - Buchi reaction – Photo oxidation – photo reduction.

Pericyclic reactions: conservation of orbital symmetry – Electrocyclic reactions – cycloaddition reactions and sigmatropic rearrangements – applications of correlation approach, Frontier Molecular orbital approach.

Books for Reference:

- 1. DeMayo P., Molecular Rearrangements, Academic Press, London.
- 2. Gould E.S., Mechanisms and Structure in Organic Chemistry, Henry Holt and Co., New York, 1959.
- 3. Harris J.M., and Wamser C.C., Fundamentals of Organic Reaction Mechanisms, John Wiley and Sons Inc., New York, 1976.
- 4. Mukerji S.M., and Singh S.P., Reaction Mechanisms in Organic Chemistry, McMilan India Ltd. 1978
- 5. Agarwal O.P., Natural Products, Vol. I and II, Goel Publication, Meerut.
- 6. De Mayo P., Chemistry of Terpenoids, Vol. I and II, Academic Press, London.
- 7. Morrison R.T., and Boyd R.N., Organic Chemistry, Prentice Hall, 6th Edition, New Delhi, 1995.
- 8. Bellamy A.J., An introduction to Conversation of Orbital Symmetry, Longman, England, 1974.
- 9. Depuy C.H., and Chapman O.L., Molecular Reactions and Photo Chemistry, Prentice Hall, New Delhi, 1972.
- 10. Finar I.L., Organic Chemistry Vol.-II., ELBS, England, 1975.
- 11. Ireland R.E., Organic Synthesis, Prentice Hall of India (P) Ltd, New Delhi, 1975.
- 12. March J., Advanced Organic Chemistry, Wiley, 6th Edition, New York, 2007.

II YEAR – III SEMESTER COURSE CODE: 7MCH3C2

CORE COURSE-X-INORGANIC CHEMISTRY-III

Objectives:

- To enable the students in-depth study of spectral applications to the structural elucidation of inorganic compounds.
- To know the details of lanthanides and actinides.

Unit I: Application of IR, Raman and Mossbauer Spectroscopy to the Study of Inorganic Compounds

[15 hrs]

Application of IR and Raman spectra in the study of coordination compounds – application to metal carbonyls, nitrosyls and sulphate – geometrical and linkage isomerism – detection of inter and intramolecular hydrogen bonding.

Mossbauer Spectroscopy: Mossbauer Effect – resonance absorption – Doppler effect – Doppler velocity – isomer shift –magnetic hyperfine splitting-application of Mossbauer spectroscopy in the study of iron and tin complexes.

Unit II: Electronic Spectra and NMR Spectroscopy of Inorganic Compounds

[15 hrs]

d-d transition – charge transfer transition – selection rules – mechanism of beak down of selection rules – bandwidths and shapes – Jahn Teller effect – Orgel diagram - evaluation of 10Dq and β for octahedral and tetrahedral complexes.

NMR Spectroscopy: ³¹P and ¹⁹F and – NMR spectroscopy – Introduction – application in structural problem – evaluation of rate constants – monitoring the course of reaction – NMR of fluxional molecules – NMR of paramagnetic molecules – contact shifts and shift reagents.

Unit III: Metallurgy and Complexes

[15 hrs]

Occurrence, isolation, purification, properties and uses of the following metals as well as their important compounds: Be, Ge, Pb and Se.

Complexes of π - acceptor ligands: Synthesis, properties, structure and bonding in mononuclear and dinuclear metal carbonyls – Application of EAN rule. Synthesis, properties, structure and bonding in Ferrocene complexes – magnetic properties.

Unit IV: Lanthanides and Actinides

[15 hrs]

Lanthanides: Occurrence – separation techniques (precipitation, ion-exchange, solvent-extraction and Selective reduction and oxidation) – Electronic configuration – Oxidation states, Lanthanide contraction – Spectral and Magnetic properties- Lanthanides as shift reagents in NMR – uses of lanthanides and their compounds – position in the periodic table.

Actinides: Synthesis of elements – Extraction of Th, U and Pu from fission products-electronic configuration and oxidation states, spectral and magnetic properties – position in the periodic table.

Unit V: Cages and metal clusters

[15 hrs]

Electron deficient compounds: Borane and carboranes – nomenclature – Synthesis, properties, structure and bonding in diborane and tetraborane – wades rule – Styx numbers.– Synthesis, properties and structure of Ferrocene.

Metal clusters: Polyacids – classification of polyacids – synthesis, structure and bonding in poly anions and isopoly anions of phosphorous, Molybdenum and tungsten.

Books for Reference:

- F.Basalo and R.G. Pearson, Mechanism of Inorganic Reactions, 2nd End., Wiley New York, 1973
- 2. R.S Drago, Physical Methods in Chemistry, Saunder Golden Sunburst Series, W.B. Saunders company; London 1977.
- 3. Raymond Chang- Basic principles of Spectroscopy, Mc Graw Hill, New Delhi. 1971.
- 4. Nakamoto, Kazuo, Infrared and Raman Spectra of Inorganic and coordination compounds, IV edition, John Wiley and Sons, New Yark, 1986.
- 5. J.D.Woolings, Non Metal Rings, Cages and Clusters, John Wiley and sons, New York, 1989.
- 6. R. S. Drago, Physical Methods in Inorganic Chemistry; Affiliated East-West Press Pvt. Ltd., New Delhi, 2012.
- 7. W. Kemp, Organic Spectroscopy; 3rd Ed., Palgrave, New York, 2011.
- 8. Wahid U.Malik, G.D. Tuli and R.D.Madan, Selected Topics in Inorganic Chemistry, S.Chand & Co. Ltd., New Delhi, 2006.
- 9. Douglas and McDaniel, A Concise of Inorganic Chemistry, Oxford and IBH Publishing company (P)Ltd., New Delhi. 2002.
- 10. E. Huheey, Ellen A.Keiter, Richard L.Keiter, Inorganic Chemistry, IV Edn., Pearson Education (Singapore) Pte.Ltd., Delhi, 2004.
- 11. William W. Porterfield, Inorganic Chemistry, Elsevier, II Edn., New Delhi. 2005.
- 12. A.G. Sharpe, Inorganic Chemistry, Addition Wesley Longman, UK III Edn., 2004.
- 13. Gary L. Miessler and Donald A. Tarr, Inorganic Chemistry, Pearson Education, Inc., 3rd Edn., New Delhi. 2004.
- 14. D.N. Sathyanarayana, Electronic Absorption Spectroscopy and Related Techniques, Universities Press (India) Limited, 2001.



II YEAR – III SEMESTER COURSE CODE: 7MCH3C3

CORE COURSE-XI-PHYSICAL CHEMISTRY-III

Objectives:

Unit I: Photo and Radiation Chemistry

[15 Hrs]

Physical properties of the electronically excited molecules – Photophysical Process – Jablonski's diagram – radiationless transitions – Internal conversion and intersystem crossing – Stern-Volmer equation and its application – radiative transition – fluorescence, phosphorescence and other deactivation processes. Effect of temperature on emission process – photosensitization and Chemiluminescence – elementary aspects of photosynthesis – photochemical conversion and storage of solar energy – Experimental techniques in photochemistry – Chemical actinometers. Photochemical Kinetics of H₂-X₂ reactions.

Unit II: Quantum Mechanics – I

[15 Hrs]

Planck's explanation about black-body radiation – de-Broglie's concept of matter waves, Compton effect – Heisenberg's uncertainty principle and complementarily. Operators – Linear operators – Method of getting the following quantum mechanical operators – position, momentum, Kinetic energy, potential energy, total energy, angular momentum and spin angular momentum. Postulates of quantum mechanics – Hermicity and proving the quantum mechanical operators are Hermitian – Commutators algebra – evaluation of commutators – vanishing and non – vanishing commutators.

Unit III: Quantum Mechanics – II

[15 Hrs]

Eigen function and Eigen Value – Expansion theorem – Orthogonality and normalization of wave functions. Derivation of Schrodinger wave equation – application of SWE to simple systems – free particle moving in one dimensional box – Characteristics of wave function – average momentum of a particle in a box is zero-particle moving in a 3-D box – degeneracy – distortion – particle moving in ring – rigid rotator.

Unit IV: Application of Quantum Mechanics

[15 Hrs]

Spherical harmonics – simple harmonic oscillator – Hermite polynomials – radial wave function – radial probability distribution – shapes of various atomic orbitals. Schrodinger equation for Helium atom and other many electron system. Necessity for approximation methods – Variation methods for the Hydrogen atom – Perturbation (first order) method to Helium atom - Slater determinant wave function – secular determinant – HMO π -electron theory of Ethylene and Butadiene.

Unit V: Fast Reactions, Catalysis and Kinetic theory of gas [15 Hrs]

Catalysis: General Characteristics of Catalysis - Homogeneous Catalysis - Acid-Base Catalysis - Enzyme Catalysis - Derivations of Michaelis & Menton Equation - Heterogeneous Catalysis - Surface reactions - Kinetics of Surface reactions.

Fast reactions – flow and relaxation techniques, Temperature Jump and pressure jump method (Pulse method) – Flash photolysis.

Equations of states – Maxwell-Boltzmann distribution law – Principle of equipartition of energy and heat capacity – Rotation, vibrations and translational degree of freedom – Molecular collisions – Mean free path – transport properties – thermal conductivity.

Books for Reference:

- 1. A.K. Chandra, Introductory Quantum Chemistry, 4th Edn., Tata Mc Graw Hill Publishing Co, New Delhi, (2006).
- 2. R.K. Prasad, Quantum Chemistry, Revised 3rd Edn , New Age International Publishers, New Delhi (2009).
- 3. James.E. House, Fundamentals of Quantum Chemistry, 2nd Edn., Elsevier Publishers India Pvt. Ltd, New Delhi (2005).
- 4. IRA N.Levine Quantum Chemistry, 5th Edn., Prentice Hall of India Pvt. Ltd, New Delhi (2006).
- 5. K.K.Rohatgi Mukherjee, Fundamentals of Photochemistry, Wiley Eastern.
- 6. P.W. Atkins, Molecular Quantum Mechanics, 5th edn. Oxford University Press, (2012).



II YEAR – III SEMESTER COURSE CODE: 7MCH3P1

CORE COURSE-XII-PHYSICAL CHEMISTRY PRACTICAL-I

Objectives:

I. Conductometric Experiments

- i) Double displacement & acid base titration
 - a) NH₄C1 NaOH Mixture of CH₃COOH & HCl
 - b) NH₄C1 NaOH Mixture of NH₄C1 & HCl
- ii) Precipitation titration
 - a) $KCl AgNO_3 KCl$
 - b) $K_2SO_4 BaC1_2 K_2SO_4$
- iii) Determination of dissociation constant of weak acids.
- iv) Determination of equivalent conductance of weak electrolyte at infinite dilution using Kohlraush law.

II. Adsorption Experiments

Adsorption of Oxalic acid / Acetic and on charcoal.

III. Kinetic Experiments

- i) Kinetics of alkaline hydrolysis of ester by conductometric method
- ii) Perdisulphate and iodide ion reaction: study of Primary salt effect and determination of concentration of given KNO₃.

IV. Potentiometric methods

- i) Precipitation titration: Ag Vs halide mixture
- ii) Redox titration: a) permanganate Vs iodide ion b) Ceric ammonium Sulphate Vs ferrous ion
- iii) Determination of dissociation constant of weak acids and pH of buffer solutions.
- iv) Determination of solubility product of sparingly soluble salts.

V. Titrations using pH meter

Determination of first, second and third dissociation constants of phosphoric acid.

Book for Reference:

1. J.B.Yadav; "Advanced Practical Physical Chemistry" 6th Edn., Goel Publications, Meerut, 1986.

II YEAR – III SEMESTER COURSE CODE: 7MCH3E1

ELECTIVE COURSE-III (A)-PHARMACEUTICAL CHEMISTRY

Objectives

To enable the learners to know the fundamentals of pharmaceutical Chemistry, concept of chemotherapy and its agents.

Unit I: Introduction to Drug and drug design

[15 Hrs]

Historical background-sources and classification of drugs-important terminologies in pharmaceutical chemistry. Concept of drug, lead compound and lead modification, prodrugs and soft drugs.

Structure-activity relationship (SAR) and the development of Quantitative Structure Activity Relationship (QSAR). Factors affecting bioactivity – resonance, inductive effect, isosterism, bio-isosterism, spatial considerations; Theories of drug activity – occupancy theory, rate theory, induced fit theory Concept of drug receptors – elementary treatment of drug-receptor interactions; Physicochemical parameters – lipophilicity, partition coefficient, electronic ionization constants, steric, Shelton and surface activity parameters and redox potentials;

Pharmacokinetics and pharmacodynamics: administration, absorption, distribution, medicinal chemistry.

Unit II: Antibiotics & Antivirals

[15 Hrs]

Structural features and SAR of the following antibiotics – penicillin G, cephalosphorin and their semisynthetic analogs (β – lactam), streptomycin (amino glycoside), terramycin (tetracycline), erythromycin (macrolide) and chloramphenicol. Synthesis of penicillin-V and Chloramphenicol.

Anti-AIDS and Anti-viral agents (A brief study and medicinal importance), Antimalarials - Classification Synthesis of Chloroquine

Unit III: Antineoplastic agents & Psychoactive drugs

[15 Hrs]

Introduction, cancer chemotherapy, role of alkylating agents and antimetabolites in treatment of cancer. Synthesis of antineoplastic agents viz. Mechlorethamine, cyclophosphamide, chlorambucil and 6- mercaptopurine.

Introduction, neutotransmitters, CNS depressants, general anaesthetics, mode of action of hypnotics, sedatives, neurochemistry of mental diseases.

Unit IV: Cardiovascular Drugs

[15 Hrs]

Cardiovascular Drugs and Local Antiinfective Drugs: Introduction, Cardiovascular diseases, drug inhibitors of peripheral sympathetic function, central intervention of cardiovascular output.

Synthesis of cardiovascular drugs viz. amyl-nitrate, sorbitrate, methyldopa, verapamil and atenolol.

Unit V: Analgesics, anaesthetics and antihypertensive drugs

[15 Hrs]

Narcotic analgesics: Analgesic action of Morphine. Synthetic analgesics: pethidine. Non-Narcotic analgesics-aspirin, methyl salicylate, paracetamol and phenacetin

General anaesthetics-Volatile general anaesthetics, Intravenous anaesthetics or non-volatile anaesthetics. Local anaesthetics-Classification.

Synthesis and therapeutic action of Nifedipine, captopril, hydralazine, sodium nitroprusside, clonidine and guanothidine.

Books for Reference:

- 1. Goodman & Gilman. Pharmacological Basis of Therapeutics, McGraw-Hill (2005).
- 2. S. S. Pandeya & J. R. Dimmock.Introduction to Drug Design, New Age International.(2000).
- 3. Graham & Patrick. Introduction to Medicinal Chemistry (3rd edn.), OUP (2005).
- 4. Finar, I. L. & Finar, A. L. Organic Chemistry Vol. 2, Addison-Wesley (1998)
- 5. Finar, I. L. Organic Chemistry Vol. 1, Longman (1998)
- 6. Gringauz, A. Introduction to Medicinal Chemistry: How Drugs Act and Why? John Wiley & Sons (1997).
- 7. Patrick, G. L. Introduction to Medicinal Chemistry Oxford University Press (2001).
- 8. S.S.Pandeya and J.R.Dimmock, An Introduction to Drug Design, New Age, International, 2006.
- 9. Introductory Medicinal Chemistry, J.B.Taylor and P.D.Kennewell, Ellisworth publishers, 1985
- 10. Fundamentals of Medicinal Chemistry by Gareth Thomas, John Wiley & Sons: Chichester, 2003.
- 11. Medicinal Chemistry: An Introduction by Gareth Thomas, Wiley-Interscience, 2nd edition, 2008.
- 12. An introduction to Medicinal Chemistry by Graham L. Patric, Oxford University Press, USA, 3rd edition, **2005**.
- 13. Wilson and Giswald's Textbook of Organic Medicinal and Pharmaceutical Chemistry by John Block and John M Beale (Eds), Lippincott Williams & Wilkins, 11th edition, **2003**.
- 14. The Organic Chemistry of Drug Design and Drug Action by Richard B. Silverman, Academic press, 2nd edition, 2004.
- 15. Jayashree Ghosh, A textbook of Pharmaceutical Chemistry, S.Chand & Company Ltd., New Delhi, 2012.

II YEAR – III SEMESTER **COURSE CODE: 7MCH3E2**

ELECTIVE COURSE-III (B)-MATERIAL CHEMISTRY

Objective

To understand the basic concept of Structure of matter and their various properties.

Unit I: Structure of Matter

[15 Hrs]

Atomic structure: Wave mechanical model; electronic configurations; ionic, covalent, metallic and secondary bond. Space lattices and crystal ographic systems; influence of radius ratio on coronation, structure of common metallic, semi conducting, ionic, polymeric and ceramic materials.

Use of X-ray diffraction for determination of simple structures, point, line and surface defects; geometry of edge and screw dislocations. Burger's vector; grain and twin boundaries.

Unit II: Polymeric Materials and its mechanical properties [15 Hrs]

shape, structure and configuration, crystallinity, stress- strain Molecular behavior, thermal behavior, polymer types and their applications, conducting and ferroelectric polymers.

Elastic, anelastic and viscoelastic behaviours of materials, atomic model of elastic behaviours, rubber - like elasticity, relaxation processes, displacement model for viscoelasticity, plastic deformation, slip systems in crystals, critical resolved shear stress, work hardening, strengthening mechanism, ductile and brittle fracture, Griffith's criterion; failure of materials due to creep and fatigues, deformation behaviours of polymers and ceramics.

Unit III: Ceramics, Composites and Nanomaterials Liquid Crystals. [15 Hrs]

Ceramics, Composites and Nanomaterials: Ceramic structures, mechanical properties, clay products. Refractories, characterization, properties and applications. Microscopic composites, dispersionstrengthened and particle-reinforced composites, macroscopic composites. Nanocrystalline phase, preparation procedures, properties and applications.

Liquid Crystals: Thermotropic liquid crystals, positional order, bond orientational order, nematic and smectic mesophases. Molecular arrangement in smectic A and smectic C phases, optical properties of liquid crystals. Dielectric susceptibility and dielectric constants. Lyotropic phases and their description of ordering in liquid crystals.

Unit IV: Magnetic, Optical and thermal properties Magnetic properties

[15 Hrs]

Magnetic behaviours of materials: dia, para, ferro and ferri magnetisms, soft and hard magnetic materials including ceramic magnets,

Optical Properties

Optical properties of materials, elementary ideas about absorption, transmissions and reflection refractive index, lasers and their application, optoelectronic devices.

Thermal properties

Thermal properties of materials, specific heat, thermal conductivity and thermal expansions.

Unit V: Organic Solids & Ionic conductors

[15 Hrs]

Organic Solids:Fullerenes, Molecular Devices. Conducting organics, organic superconductors, magnetism in organic materials. Fullerenes, doped, fullerenes as superconductors. Molecular rectifiers and transistors, artificial photosynthetic devices, optical storage memory and switches, sensors. Non-linear optical materials, non-linear optical effects. Molecular hyperpolarisability.

Ionic conductors: Types of ionic conductors, mechanism of ionic conduction, interstitial jumps (Frenkel); vacancy mechanism, diffusion superionic conductors, phase transtions and mechanism of conduction in superionic conductors. Examples and applications of ionic conductors.

Books for Reference:

- 1. V.Raghavan, A First course in Materials science and Engineering, Prentice-Hall of India Private Ltd., New Delhi.
- 2. A.G.Guy, Elements of Materials Science Mc Graw Hill.
- 3. A.L.Ruoff, Introduction to Materials Science, Prentice-Hall.
- 4. M.F.Ashby and D.R.H,Jones, Engineering Materials, Pregamon
- 5. O.P.Khana, A Text book of Material Science and Metallurgy, Damphat Rai &Sons, New Delhi.
- 6. C.M.Srivastava & C.Srinivasan, Science of Engineering Materials, New Age International (P) Ltd., New Delhi.
- 7. C.Kittd, Solid State Physics, Wiley Eastern Ltd., 1995.
- 8. B.S.Saxena R.C.Gupta and P.M. Saxena, Fundamentals of Solid State Physics, Pragati Prakasham Educational Publishers, Meerat
- 9. K.L Chopra and I.Kaur, Thin Film Devices and Their Applications, Plenum Press, New York, 1983.
- 10. K.S.V.Santhanam and M.Sharon, Photoelectrochemical solar cell, Elsevier Science Publishers, New York, 1988.
- 11. A.F.Fahrenbruch and R.H. Bube, Fundamentals of solar cells. Academic Press. London 1081.
- 12. J. C. Anderson , K. D. Leaver, J. M. Alexander and R D.Rawlings, Materials Science. ELBS



II YEAR – IV SEMESTER COURSE CODE: 7MCH4C1

CORE COURSE-XIII–INSTRUMENTAL METHODS OF ANALYSIS

Objectives:

Zero To enable the learners to learn the principle of electro analytical methods & spectroanalytical methods.

Unit I: Error Analysis

[15 Hrs]

Error analysis: Classification of errors – accuracy and precision – minimization of errors –significant figures – significant figures in computation – statistical treatment of data: mean, median, standard deviations, variance, relative standard deviation – spread, errors – standard deviation of computed results – Student's t-test – F-test – comparison of the means of two samples – correlation and regression: linear regression (least square analysis).

Unit II: Precipitation Techniques

[15 Hrs]

Introduction – properties of precipitates and precipitating reagents – colloidal precipitates. Co–precipitation – post precipitation – precipitates from homogeneous solution – surface adsorption – drying and ignition of precipitates – application of gravimetric methods.

Unit III: Electro analytical methods

[15 Hrs]

Electro analytical techniques: Electro gravimetry, theory of electro gravimetric analysis – electrolytic separation and determination of metal ions. Coulometry: Electrolytic cell – working electrodes – auxiliary electrode and reference electrode – coulometric titrations. Voltammetry: stripping voltammetry – chronopoteniometry: Amperometry: Amperometric titrations.

Unit IV: Thermo analytical Methods

[15 Hrs]

Thermal analysis, theory and principles of DTA and TGA – factors affecting the position of DT and TG traces – application of DTA and TGA. to the thermal behavior of the following compounds – crystalline copper sulphate, calcium oxalate monohydrate, calcium acetate monohydrate, zinc hexafluorosilicate – complementary nature of DTA and TGA – principle and application of DSC – determination of degree of conversion of high alumina cement

Unit V: Spectro analytical Methods

[15 Hrs]

Colorimetry: Beer and Lambert's law – terminology – condition for a satisfactory colorimetric analysis – method of colour measurement or comparison – principles, Instrumentation and applications of colorimetry (determinations of Cr, Cu, Fe, Mn & Ni).

Principle, Instrumentation and Applications of Turbidimetry, fluorimetry, Flame photometry and AAS.

Books for Reference:

- 1. D.A.Skoog, D.M.West and F.J.Hollar. Fundamentals of Analytical Chemistry, 7th Edition, Harcourt College Publishers, 1996.
- 2. H.H.Williard. L.L.Merritt and J.A.Dean, Instrumental Methods of Analysis, East-West press, New Delhi, 1988.
- 3. J.Basset et al., Vogel's text book of Qualitative Inorganic Analysis, Longman, 5th Edition, ELBS, Essex, 1989.
- 4. J.G.Dick, Analytical Chemistry, Tata Mc-Graw Hill, 1973.

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II YEAR – IV SEMESTER COURSE CODE: 7MCH4E1

ELECTIVE COURSE-IV – (A) – NANO CHEMISTRY

Objective

Unit I: Nanomaterials- An Introduction and Synthetic methods [15 Hrs]

Definition of nanodimensional materials - Historical milestones - unique properties due to nanosize, Quantum dots, Classification of Nanomaterials .

General methods of synthesis of nanomaterials—Hydrothermal synthesis, Solvothermal synthesis, Microwave irradiation, sol – gel and Precipitation technologies, Combustion Flame-Chemical Vapor Condensation Process, gas Phase Condensation Synthesis, Reverse Micelle Synthesis, Polymer–Mediated Synthesis, Protein Microtube–Mediated Synthesis. Synthesis of Nanomaterials using microorganisms and other biological agents, Sonochemical Synthesis, Hydrodynamic Cavitation.

Unit II: Nanostructured materials and applications of nanomaterials [15 Hrs]

Carbon Nanotubes (CNTs): Single walled carbon nanotubes (SWNTs), Multiwalled carbon nanotubes (MWNTs), Graphenes, Fullerenes, Metal/Oxide nanoparticles (NPs), Nanorods, Nanotubes and Nanofibres, Semiconductor quantum dots, Polymer NPs. Application of carbon nanotubes.

Applications of Nanomaterials in various fields: Pharmaceuticals, Medical & Health, Energy, Environment. Textiles, Water, Defence,

Unit III: Carbon Clusters, Inorganic and organic nanomaterials [15 Hrs]

Nature of carbon bond: New carbon structures—Carbon clusters: Discovery of C_{60} —Alkali doped C_{60} —Superconductivity in C_{60} —Larger and smaller fullerenes.

Inorganic nanomaterials : Typical examples –nano TiO₂ / ZnO/CdO/CdS,

Organic nanomaterials: examples – Rotaxanes and Catenanes

Unit IV: Characterization techniques for nanomaterials [15 Hrs]

Electron Microscopy: Scanning electron microscopy (SEM), Transmission electron microscopy (TEM), Scanning Probe Microscopic Techquics; Atomic force Microscopy (AFM) and Scanning Tunneling Microscopy.

Particle size Analyser (Dynamic light scattering), X-ray Differaction (XRD), Auger Emission Spectroscopy, Electron Spectroscopy for Chemical analysis (ESCA)

Unit V: Nanotechnology and nanodevices [15 H

DNA as a nanomaterial, DNA – knots and junctions, DNA – nanomechanical device designed by Seeman.Force measurements in simple protein molecules and polymerase – DNA complexes. Molecular recognition and DNA based sensor. Protein nano array, nanopipettes, molecular diodes, self assembled nano transistors, nanoparticle mediated transfection.

Books for Reference:

- 1. The Chemistry of Nanomaterials, C.N.R. Rao, A. Muller, A.K. Cheetham, Eds. WileyVCH, Germany, 2004.
- 2. Nanochemistry: A Chemical Approach to Nanomaterials, G. Ozin, A. Arsenaut, Eds, Royal Society of Chemistry, London, 2005
- 3. M-C. Daniel, D. Astruc, Gold Nanoparticles: Assembly, Supramolecular Chemistry, Quantum-size Related Properties and Applications Towards Biology, Catalysis and Nanotechnology, Chem. Rev. 104 (2004) 293-346.
- 4. Nano: The Essentials, Understanding Nanoscience and Nanotechnology, T. Pradeep, McGraw Hill Education, New Delhi, 2007.
- 5. Charles P.Poole, Jr. and Frank J.Owens; Introduction to Nanotechnology, Wiley, 2003.
- 6. G. Cao, Nanostructures and Nanomaterials: Synthesis, Properties and Applications, Imperial College Press, London, 2004.
- 7. C.M. Niemeyer and C.A. Mirkin, Nanobiotechnology, Concepts, Applications and perspectives, WILEY-VCH, Verlag Gmb H&Co, 2004.
- 8. T.Pradeep, "Nano: The essentials, Tata Mc Graw Hill, New Delhi, 2007.
- 9. Willard, "Instrumental Methods of Analysis", 2000.
- 10.T. Tang and p. Sheng (Eds), Nano Science and Technology Novel Structures and Phenomena, Taylor & Francis, New York, 2004.
- 11. A. Nabok, Organic and Inorganic Nanostructures, Artech House, Boston, 2005.
- 12. Edward A. Rietman, Molecular engineering of Nanosystems, Springer- Verlag, New York, 2001.

II YEAR – IV SEMESTER COURSE CODE: 7MCH4E2

ELECTIVE COURSE IV -(B) -CORROSION CHEMISTRY

Objective:

To understand the importance of structural metals and its alloys, to prevent the corrosion and save their life

Unit I: Basic aspects of corrosion

[15 Hrs]

Importance of corrosion studies – EMF and Galvanic series – Classification of corrosion, Dry corrosion and Electrochemical corrosion – Difference between Chemical and Electrochemical corrosion – Theory of Electrochemical corrosion – Factors influencing corrosion, Nature of the metal and Nature of the environment - Corrosion control methods – cathodic protection.

Unit II: Environmental aspects and electrolytic factors [15 Hrs]

Types of corrosion – pitting, inter-granular, Waterline corrosion, stress corrosion, erosion corrosion, Galvanic Corrosion, Dezincification and Corrosion fatigue - Atmospheric corrosion – classification, factors influencing atmospheric corrosion – Microbiological Corrosion – Corrosion failure due to activity of Micro-organisms - Underground (or) Soil corrosion.

Unit III: Protective Coatings

[15 Hrs]

Introduction – Classification – Metallic coating, Non – metallic coating and Organic coating – Pre-treatment of the surface – Metallic coatings, Hot dipping, Spraying, Cladding, Cementation – Electroplating – Process, Types of Electroplating – Factors affecting Electroplating – applications of Electroplating – Inorganic Non-metallic coating - Chromate coating, Phosphate coating and Oxide coating – Organic coating, Paints, Requirements of Good paint.

Unit IV: Energy Conversion

[15 Hrs]

Electrochemical energy conversion – thermodynamic reversibility – characteristic and performance criteria – battery terminology Gibb's equation – EMF – phenomena of polarization, batter terminology – energy density – power density – basic principles and criteria for selection of anodes and cathodes – different types of primary cells and secondary cells – applications of primary and secondary cells – types of electrolytes – aqueous, non-aqueous, molten salt and solid electrolytes

Unit V: Fuel cells [15 Hrs]

Introduction – types of fuel cells, advantages – thermodynamics and efficiencies – electro catalysis of hydrogen oxidation and oxygen reduction – porous electrodes. Types, current – voltage relationship – limiting current density, mercury porosimetry. Various fuel cell systems – alkaline, phosphoric acid, molten carbonate, solid oxide and solid polymer fuel cell systems.

Books for Reference:

- 1. D.Pletcher and F C Walsh, Industrial Electrochemisty, Vol.II, Blakrid Academic Professional, London, 1993.
- 2. D.Jones, Principles and prevention of corrosion, Macmillan Publications, New York 1992.
- 3. J J Meketta, Cathodic protection Theory and practice, Marcel Dekker Publication, New York, 1993.
- 4. S N Banerjee, An introduction to corrosion and corrosion inhibition, oxonian press Ltd., New Delhi.
- 5. L L Shrier, Corrosion Vol I & II Goege Nouns Ltd., Southampton Street, London.
- 6. M G Fonlana & N D Greene, Corrosion Science and Engineering, McGraw Hill Book Co., New York.

II YEAR – IV SEMESTER COURSE CODE: 7MCH4E3

ELECTIVE COURSE-V- (A) – GREEN CHEMISTRY

Objective

Unit I: Introduction to Green Chemistry

[15 Hrs]

The need for green chemistry–sustainability and cleaner production-eco efficiency–environmental protection laws, challenges ahead for a chemist–Education on Green chemistry–Dreaming green chemistry-Innovations for a cleaner world-Pollution-a prize tag of modern society-From Pollution control to pollution prevention- Green chemistry-the need of the day-Green methods-green products, recycling of waste.

Unit II: Introduction, Inception and evolution of Green chemistry [15 Hrs]

Introduction, twelve principles of green chemistry-explanation of the twelve principles of green chemistry-Atom economy-Scope of Green chemistry-inception of green chemistry-awards for green chemistry-international organizations promoting green chemistry.

Unit III: Adverse effects of chemicals on health and environment

[15 Hrs]

Health and environment—heavy metals—arsenic—methods of removing arsenic from water, mercury, cadmium vanadium, uranium, beryllium, health impacts of lead, manganese, cobalt, nickel, thallium, tellurium and selenium.

Unit IV: Designing Green Synthesis

[15 Hrs]

Green Synthesis: Designing, Choice of starting materials, choice of reagents, choice of solvents, choice of catalyst.

Organic synthesis in water: Reactions in water-Claisen rearrangement, Knoevenagel reaction, Pinacol coupling, Benzoin condensation and strecker synthesis.

Ionic liquids: Types of ionic liquids, synthesis of ionic liquids-Reaction in ionic liquids-Suzuki coupling, Claisen-Schimidt condensation and Waker-type oxidation reactions.

Super critical Fluids: Introduction-Supercritical CO_2 – super critical polymerization, Kolbes-Schmitt synthesis and Friedel-Craft reaction.

Unit V: Solvent-Free organic synthesis

[15 Hrs]

Microwave assisted synthesis-microwave activation, microwave heating- advantages of microwave exposure and specific effects of microwaves .

Microwave assisted synthesis in water: Hoffmann elimination, hydrolysis of benzamide and oxidation of toluene

Ultrasound assisted organic synthesis: Introduction-Types of sonochemical reactions-Homogeneous sonochemical reactions-Curtius rearrangement-Heterogeneous Liquid-Liquid reactions: esterification-Heterogeneous Solid-Liquid reactions: Hydroboration.

Phase Transfer Catalysts: advantage, types and application in conversion of nitriles from akyl and aryl halides,

Biocatalyst: Microbial oxidation and enzymatic hydrolysis -polymer supported catalysts.

Books for Reference:

- 1. Paul T. Anastas Green Chemistry.
- 2. Rashmi Sanghi & M M Shrivastav Green Chemistry, Environment Friendly Alternatives. Narosa Publishing House Pvt.Ltd.,New Delhi, 2012.
- 3. V.K.Ahluwalia, Green chemistry A Text Book, Narosa Publishing House Pvt.Ltd.,New Delhi, 2013.
- 4. M.Kidwai & Ahlavalia V.K.Green Chemistry
- 5. V.Kumar, An Introduction to Green Chemistry, Vishal Publishing Co., Jalandhar, 2007.
- 6. B.K.Sharma, Environmental Chemistry, GOEL Publishing House.
- 7. Shweta Sharma and Pooja Sharma, Environmental Chemistry: Narosa Publishing House Pvt. Ltd., New Delhi, 2014.

II YEAR – IV SEMESTER COURSE CODE: 7MCH4E4

ELECTIVE COURSE -V (B) - MOLECULAR PHOTOCHEMISTRY

Objective

To understand the importance of structural metals and its alloys, to prevent the corrosion and save their life.

Unit I: Photo Physical processes

[15 Hrs]

Photo Physical processes in electronically excited molecules – Radiation less transitions – Jablonski diagram – Internal conversion and intersystem crossing. Fluorescence emission – Fluorescence and structure. Triplet states and phosphorescence emission – Photo physical kinetics unimolecular Processes.

Unit II Photo reduction and oxidation reactions

[15 Hrs]

Photo reduction and related reactions. Photo oxidation and Photo Oxygenation Nature and importance of singlet oxygen quenching on Fluorescence by oxygen. Cycle addition reactions Photo dimerisation, oxetane formation – Woodward – Hoffman rules, Chemiluminescence.

Unit III Photo Chemistry of transition metal complexes

[15 Hrs]

Photo Chemistry of transition metal complexes – Photo substitution, photo rearrangement and photo redox reactions photo chemistry of metallocenes. Applications of Inorganic Photo chemistry in photo chemical conversion and storage of solar energy.

Unit IV Photochemistry of alkenes and carbonyl compounds

[15 Hrs]

Photochemistry of alkenes and carbonyl compounds; Photooxygenation; Photochemistry of aromatic compounds; Photochemical isomerisation, addition and substitution; Photo – Fries rearrangement of ethers and anilides; Barton reaction, Hoffmann – Loefller – Freytag reaction, di- π -methane rearrangements; Singlet molecular oxygen reactions; Photo cleavages.

Unit V Experimental techniques in photo chemistry

[15 Hrs]

Experimental techniques in photo chemistry – Chemical actinometry – Ferrioxalate, uranyl oxalate, photochroic, Reinecke's salt actinometeres – Lasers and their applications.

Books for Reference:

- 1. K.K.Rohatgi Mukherjee, Fundamentals of photo chemistry. Wiley Eastern Ltd., 1988.
- 2. N.J.Turro, Molecular Photochemistry, New York W.A. Benjamin, 1966.
- 3. S. Arunachalam, Inorganic photochemistry, Kala Publications.

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II YEAR – IV SEMESTER COURSE CODE: 7MCH4PR

CORE COURSE XIV - PROJECT

Objective

Zero gain the hands on experience of different instruments and exposure of research potential.

Project Work

- 1. Each learner can select for his/her research project in any one of the areas of chemistry in consultation with his/her guide and the Head of the Department.
- 2. The Project report should be submitted to the Principal through the Head of the Department of Chemistry on or before 31st March of every year.
- 3. Each learner shall submit 2 copies of his/her project report for Evaluation.
- 4. The project report shall contain at least 25 pages excluding bibliography and appendices.
- 5. A Candidate shall be declared to have passed in each course if he / she secures not less than 40% marks in the University Examinations and 40% marks in the Internal Assessment and not less than 50% in the aggregate, taking Continuous assessment and University Examinations marks together.
- 6. The candidates are not permitted to improve their Internal Assessment marks.
- 7. A Candidate shall be declared to have passed in the Project Work if he / she gets not less than 40% in each of the Project Report and Viva Voce but not less than 50% in the aggregate of both the marks for Project Report and Viva Voce.
- 8. A candidate who gets less than 40% in the Project Report must resubmit the Project Report. Such candidates need take again the Viva Voce on the resubmitted Project.

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