Project Chemistry

Department of Chemistry

Paper I - Biomolecules, Rearrangements and Synthetic Methods

Unit I : Carbohydrates, Amino acids, proteins and Nucleic acids :

Classification of proteins – peptides – structure of peptides - synthesis of peptides – Chemisty of gluthathione and oxytocin – an elementary treatment of enzymes, coenzyme and nucleic acids – biosynthesis of amino acids – RNA and protein synthesis – Genetic code – DNA and determining the base sequence of DNA.

Pyronose and furanose, forms of aldohexoses and keto hexoses – methods used for determination of ring size – conformations of aldohexopyranoses – structure and synthesis of maltose, lactose, sucrose and cellobiose. A brief study of starch and cellulose.

Unit II : Photochemistry & Free radicals :

Conservation of orbital symmetry – electrocyclic reactions – cyclo addition reactions and sigmatropic rearrangements – applications of correlatioin diagram approach frontier molecular orbital approach, Huckel Mobius approach and Perturbation molecules orbital approach to the above reactions.

Photochemical reactions of ketones – photosensitization – Norrish I and Norrish type reactions – paterno – Buchi reaction – photooxidation – photoreduction – photochemistry of arenes.

Free radicals : Formation, detection and stability of free radicals – free radical reactions halogenations, addition, oxidation, reduction and rearrangement reactions – BartoSandmeye, Gomberg, Bachmann, Ultmann, Pschorr and Hundsdiecker reactions.

Unit III Molecular rearrangements

Mechanism of the following rearrangemetns reactions : Wagner - Meerwein, Pinacol, Demzanov. Beckmann, HOffmann, Curtius , Wolff, Baeyer - Villeger, Stevans, Sommelet – Hauser , Favorskii, Banzil – benzilic acid, Claisen, Cope, Fries, Dienone – phenol, di-pimethane, hydroxioamino – p=aminophenol and Benzidine rearrangement - Photochemical arrangements.

Unit IV Green Chemistry – I

Principles of green chemistry – planning a green synthesis in a laboratory - general interest for solvent free processes – solvent free techniques – Microwave synthesis : Introduction and characteristics of microwave heating – interaction of microwave radiation with the material – difference between conventional heating and microwave heating. Dielectric polarization – dipolar polarization - applications and advantages of microwave heating over conventional heating.

PRINCIPAL
Arulmigu Palaniandavar College
of Arts & Culture.
PALANI-624601.

Unit – V Synthetic methods

Planning a synthesis - Relay approach and convergent approach to total synthesis Retrosynthetic analysis of simple organic compounds – functional group interconversions - use of activating and blocking groups in synthesis – stereoselective problems of geometrical and optical isomerism – steric crowding – Transition metal complexes in organic chemistry – Homogeneous hydrogenation – Regioselectivity – Disastereoselectivity – Enantioselectivity – Umpolung synthesis – Robinson annelation – A schematic analysis of the total synthesis of the following compounds; 2,4, dimethyl 1-2 –hydroxypentanoic acid, trans – 9 –methyl – 1- decalone and isonootkatone.

PRINCIPAL
Arulmigu Palaniandavar College
of Arts & Culture.
PALANI-624601.

Chemical kinetics, Surface, Biophysical and Photochemistry

Unit I : Chemical kinetics I: Empirical rate laws – influence of temperature on the rate of reaction – Theories of reaction rates – Arrhenius theory , collision theory and transition state theory of reaction rates – potential energy surfaces – kinetic isotope effect- Theory of unimolecular reactions – Lindemanns theory , Hinshelwood theory , RRK theory, RRKM theory and slaters theory – chain reactions – steady state approximations – kinetics of chain reactions – thermal reaction between H_2 and Br_2 – thermal decomposition of N_2O_5 and acetaldehyde – H_2 – O_2 explosive reactions. Reaction in solutions – influence of solvent dielectric constant , ionic strength – Bronsted – Bjerrum equation – primary and secondary salt effect – effect of pressure on reaction rates – significance of volume activation.

Unit II : Chemical Kinetics II and Catalysis : Fast reactions – Fast reactions techniques – flow methods (Continous and stopped flow methods) – relaxation methods (T and P jump methods) – pulse techniques (Pulse radiolysis , flash photolysis) – shock tube method – molecular beam method – life time method – Homogeneous catalysis – acid base catalysis – vant Hoff and Arrhenious intermediates for protolytic and prototropic mechanism. Catalysis in Biological systems- enzyme catalysis – Michaelis – Menten kinetics – Lineweaver and Burk plot
– Eadie plot – influence of pH on the enzyme catalysis. Heterogeneous catalysis – kinetics and mechanism of unimolecular and bimolecular reactions – Langmuir – Hinshelwood and Langmuir – Rideal mechanism – ARRT of surface reactions – NH_3 synthesis , hydrogenation of C_2H_4 and cracking of hydrocarbon.

Unit III: Surface chemistry: Introduction – adsorption of gases on solid – physisorption and chemisorption – adsorption isotherms – Freundlich – longmuir – BET – Temkin adsorption isotherms, Adsorption on liquid surface – surface tension – Gibbs absorption isotherm – surface area determination – solution and interfacial behavior of surfactant – Definition and classification of surfactants – preparation of LB films- Micelles – critical micelles concentration (CMC) – structure – bimolecular reaction occuring in a micellar solution – reverse micelles – micro emulsion – Application of photo electron spectroscopy – ESCA and Auger spectroscopy to the study of surfaces.

Unit IV : Biophysical chemistry : Thermodynamics in biology – concept of irreversible thermodynamics – standard free energy, entropy and chemical potential change in biochemical reactions – Energy flux – Onsager reciprocal relationship – Bioenergetics and metabolism – catabolism – anabolism – energy relationship between catabolic and anabolic path ways. High energy metabolites – ATP and its role in bioenergetics – phosphoryl group transfers and ATP – Role of single oxygen in biology – Biophysical application of Mossbauer effect – Mossbauer effect in hemoglobin – spin labeling –molecular recognition. Introduction to supra - molecular chemistry and photochemistry

PRINCIPAL
Arulmigu Palaniandavar College
of Arts & Culture.
PALANI-624601.

Unit V: Photo and Radiation chemistry: Absorption and emission of radiation - Physical properties of the electronically excited molecules – excited state dipole moments, Pka and redox potentials – photo – physical processes in electronically excited molecules – Fluorescence. Phosphorescence and other deactivation processes. Excimer and Exciplex complex formation. Stern – volmer equation and its applications – Electronic energy transfer mechanisms – photosensitization and chemiluminescence. Experimental techniques in photochemistry – light sources –chemical actinometry – measurement of quantum efficiency – photosynthesis – PSI and PSII – photochemical conversion and storage of solar energy.Radiation chemistry – Source of high energy – interaction of high energy radiation with matter radiolysisof water – determination of G-value – mode of reactions of hydrated electrons – Experimental techniques of radiation chemistry – Dosimetry – Application of radiation chemistry in biology and industry.

PRINCIPAL
Arulmigu Palaniandavar College
of Arts & Culture.
PALANI-624601.

Nuclear Chemistry, Electroanalytical and Thermal Methods

Specific Objectives: To introduce the nuclear and analytical chemistry concepts, data analysis and computers in chemistry.

Learning Outcomes: Ensures the students to understand the structure of nucleus, nuclear fission and fusion, radioactivity of isotopes, electroanalytical, thermoanalytical, spectroanalytical methods. In addition the students must have knowledge of computers in chemistry, internet, browsing and searching a website.

Unit I: Structure of Nucleus and Radioactive Decay

Composition of the nucleus – nuclear size, shape and density – principal, radial and magnetic quantum numbers – magnetic and electric properties of nucleus – elementary treatment of shell (independent particle) model – nuclear configuration – parity and its conservation – mass defect and binding energy – nuclear forces theory.

Radioactive decay: Group displacement law – decay series – rate of disintegration – half life – average life – units of radioactivity – secular and transient equilibria – theories of alpha decay, beta decay, gamma emission, positron decay, nuclear isomerism, internal conversion and electron capture – Auger effect.

Unit II: Nuclear fission and Fusion and application of radioactive isotopes

Bethe's notation of nuclear process – nuclear reaction energies (Q value) – fission – energy release in nuclear fission – mass distribution of fission products – theory of nuclear fission – fissile and fertile isotopes – energy from nuclear fusion – thermonuclear reactions in stars – classification of reactors – power nuclear reactor – breeder reactor – nuclear reactors in India.

Applications of radioactive isotopes: characteristics of tracer isotopes – chemical investigations – age determination – medical field – agriculture – industry – analytical applications – isotope dilution analysis – neutron activation analysis – biological effects of radiation – waste disposal management

Unit III :Electoanalytical&Thermoanalytical methods: Electroanalytical Techniques:

Electrogravimetry: Theory of electrogravimetric analysis – electrolytic separation and determination of metal ions. Coulometry: Electrolytic cell-working electrodes – auxiliary electrode and reference electrode – Coulometric titrations. Voltammey: Cyclic voltammety – Stripping voltammetry – Chronopotentiometry, Amperometry: Amperometric titrations.

Thermoanalytical Methods: Theory, Instrumentation and applications of thermogravimetry – Differential Thermal Analysis and Differential Scanning calorimetry- Factors affecting TG and DTA curves – Difference between DTA and DSC.

Unit IV: Spectroanalytical Methods and Data handling

i) Spectroanalytical methods: Law of absorption and quantitative law of luminescence – principles and applications of spectrophotometry, fluorimetry, nepheleometry and turbidimetry – Emission spectroscopy and flame spectroscopy – atomic absorption, atomic emission and atomic fluorescence spectroscopy. Optical rotatory dispersion and circular dichroism.

PRINCIPAL
Arulmigu Palaniandavar College
of Arts & Culture,
PALANI-624601.

ii) Data Analysis: Significant figures and Significant figures in Numerical computations-Mean and standard deviation, significant figures and computation – comparison of results – F-Test and Student's t test – Rejection of results – Q Test – Correlation coefficient and linear regression - method of least square.

Unit V: Computer in Chemistry:

History and development of computers, Mainframe, micro and Super computer systems – CPU and other peripheral devices – Evolution of proramming languages: Machine language, assembly language and higher level language.

Internet – History of internet – applications of internet in Chemistry – websites in Literature Survey in Chemistry – popular websites and data bases in Chemistry– downloading the attachment / PDF files – opening, browsing and searching a website – literature searching online.

Email: Introduction – working way – mailing basics – e.mail ethics – advantages and disadvantages – creating e-mail id – receiving and sending e-mails.

PRINCIPAL
Arulmigu Palaniandavar College
of Arts & Culture.
PALANI-624601.

Quantum, Nano and macromolecular chemistry

Unit I: Quantum mechanics – An Introduction : Failure of classical mechanics and the success of quantum theory in explaining block body radiation. Photo electric effect – Bohrs theory of hydrogen atom – hydrogen spectra – Compton effect – de- Broglies concept of matter waves – distinction between matter waves and electromagnetic radiation – experimental verification of matter waves – Heisenbergsuncertainity principle – Hypothetical (gedenkan) experiments of Heisenberg – Bohrs complementarity principle. Postulates of quantum mechanics – operator algebra – Expressions – addition, subtraction and multiplication – linear operators – Laplacian operator – vector operator – ladder operator- quantum mechanical operator for the following observables : position, linear momentum , kinetic energy , potential energy , total energy and angular momentum.Commutate algebra – evaluation of commutators.

Unit II : Application of quantum mechanics to simple system: Derivation of Schrodinger wave equation- Application of SWE to simple system – particle moving in one dimensional box quantization of energy – characteristics of wave functions , probability of a particle, component of momentum, uncertainty principle through one dimensional box and electronic transition selection rule. Particle moving in three dimensional box- concept of degeneracy and distortion – Rigid rotator – rotational energy levels – simple harmonic oscillator – zero point energy – Hydrogen atom problem – Radial wave functions – radial probability distribution – shapes of various atomic orbitals – Term symbols – L -S & J-J coupling schemes – spectroscopic states.

Unit – III Approximation methods in Quantum mechanics : Need for approximation methods – the perturbation theory (first order only) – application of theperturbation method to Hydrogen and the He atom – the variation method – application of variation method to Hydrogen and He atom. Hartree – Fockselt consistent field (HFSCF) method – application to He atom – Electron spin and pauli principle – Anti symmetric nature of the wave functions – slater determinants – approximate wave function of many atoms – Molecules – Born – oppenheimer approximation- molecular Hamiltonian operators – VB treatment to hydrogen molecule – Coloumbic integral – exchange integral and overlap integral – MO treatment of hydrogen molecular cation, homonuclear and hetronuclear diatomic molecules – Molecular term symbol. Hybridisation – HMO theory – ethylene and butadiene

Unit IV : Chemistry of nano- materials: Definition and historical perfective , Effect of nano science and nanotechnology in varions fields. Synthesis of nanoparticles by chemical routs. Microscopic techniques for the characterization of nanomaterials- UV
– visible and fluorescence spectroscopy - AFM, SEM , TEM , X-ray diffraction and Microanalysis.

Unit V :Macromolucules : Polymer – definition – types of polymers – properties of polymers – kinetics and mechanism of free radical , ionic , condensation and zeigler – natta polymerization processes. Emulsion and suspension polymerization techniques – polymer molecular weight distribution – molecular weight determination – osmotic pressure method – light scattering method – ultra centrifuge method and viscosity method. Conducting polymers – chemical structure and electronic behavior of polymers – doping of conducting polymers – polymer electrodes.

PRINCIPAL
Arulmigu Palaniandavar College
of Arts & Culture.
PALANI-624601.