Error etc: BBag

Meeting 30/9/10

Friday:

Sunday:

Analytical tech: (USR) + BM

VISVA-BHARATI

Ph. D. Course Work Syllabus
Subject: Chemistry

Spectral technique – GB

Synthetic methodology – AH

BBag, USR, BM, GB, AH, IBM, PC

Paper-I: Research Methodology and Techniques (Full Marks: 100) [40 L]

Programming: Computations; numerical methods in Fortran; Error analysis: absolute error, distribution of random errors, propagation of errors, Gussian (normal) distribution, mean, median, standard deviation, method of least squares, relative error, accuracy & precision, student's t-test, Q-test, F-test; Analytical techniques: titrimetric methods of analysis, gravimetric methods of analysis, chromatographic analysis, potentiometric methods of analysis, electrical methods of analysis (electrolysis, coulometry, polarimetry, cyclic voltametry), colorimetry and spectrophotometric analysis; Spectral techniques: principles and applications of UV, FT-IR, NMR and Mass spectroscopic techniques including spectrofluorometer; Purification techniques; Synthetic methodologies: thermal, photochemical, microwave-irradiation, ultra-sound-mediated, room-temperature, aqueous media, solvent-free techniques, catalytic effects, green methods; material science: solid-state synthetic methodologies, physical properties measurements, X-ray crystallographic characterizations, SEM, TEM, synthetic polymeric compounds, thermal and spectral analysis of polymeric compounds, molecular weight determinations, commercial polymers, magnetic properties of solids and modern methods of determination.

IBM + PC

Computer : 25 marks

Paper-II: Review Work and Seminar (Full Marks: 100)

Respective students are required to compile "Review Works" on the basis of detailed literature survey in compliance with their proposed area of research related to Ph.D. works, and the same will have to be presented for viva-voce before the Faculty members and the 'Evaluating Committee'.

Paper-III: Optional Papers (Advanced Topics on Chemistry)
(Full Marks: 100) [40 L]

[Any TWO Units to be opted ; each unit: 50 Marks (20 L)]

Unit-I: ***Advanced analytical techniques:***

USR + BM

Chromatography: Principles and Classification. Theory of column efficiency in Chromatography. Gas and High Pressure liquid Chromatography. Retention and Resolution in Chromatography. Chromatography simulation of software.

Ion-Exchange Chromatography: Ion-exchange resin- recent development, synthesis and characterization, separation of various ions.

***Solid-Phase Extraction*:** Principles and process, recent development, preparation and properties of various solid phases, extraction and separation of metal ions.

***Radio analytical techniques*:** Principles, process and application.

***Radioimmunoassay*:** Principles, specificity of immunoassays, procedure, application in bio-medical field.

Unit-2: *Characterization of paramagnetic molecules:* Basic Concepts of Magnetism: The Van Vleck Equation; Zero-field splitting; High-Spin/Low-spin Equilibrium; Polynuclear Complexes; Spin Frustration; EPR of Transition Metal Complexes; NMR of Paramagnetic Complexes.

Unit-3: *Solid state chemistry:* Solid state synthetic methods; diffusion considerations; Tamman's rule; rates of reaction; significance of lattice state for reactivity; structure-sensitive reactions; structure-insensitive reactions; Intercalation compounds of graphite characteristic properties and application; Semiconductivity and metallic conductivity of metal oxides; Electrical conductivity in one dimensional solids; Peierls distortion and band splitting; Conducting organic substances; Electrical conductivity of solid electrolytes and its application; Band structure of TiO_2-a promising green photo-catalyst-application. Basic principles of Scanning Electron Microscopy (SEM); Transmission Electron Microscopy (TEM); Atomic Force Microscopy (AFM); Scanning Tunneling Microscopy (STM) and their utilization in nanoscience.

Unit-4: *Organometallic and Supramolecular Chemistry:*
Metal alkyls, Metal-alkylidenes, Metal-alkylidynes – Synthetic routes, Bonding features, Utility in organic synthesis. Metal-alkene, alkyne, allyl, butadiene complexes, bonding features. Basic aspect of supramolecular chemistry, Self-assembly, Weak interacting forces related to supramolecular chemistry, Synthesis and application of supramolecules.

Unit-5: *Chemistry of Natural Products:* Prospects of natural products research (Introduction; Recent literature on the progress of natural products research; Present-day relevance; Interface of Chemistry and Biology; Role of natural products in development of medicinal chemistry, providing "leads"); Classes of natural products and their isolation and purification (various chromatographic methods including HPLC and HPTLC); Structural elucidation of natural products (applications of various spectroscopic techniques including UV, FT-IR, 1D- and 2D-NMR, Mass); Natural products as medicinal and agrochemical agents (bioactive natural compounds, and their potential uses in medicinal chemistry as well as agrochemicals; therapeutic importance of flavanoids, alkaloids, saponins and other significant classes of natural products; Promising 'lead' candidates in drug design and drug discovery; marine natural products and drug development; medicinal agents obtained by chemical modification of natural products; physiological effects, mode of action and metabolism of some selected natural products)

Unit-6: ***Biosynthesis of Natural Products and Biochemistry:*** Biosynthesis of natural products (biosynthesis of secondary metabolites; significant biosynthetic pathways; acetate- mevalonate pathway; skikimate pathway; the isoprenoids; biosynthesis of polyketides, terpenoids, steroids, alkaloids, phenylpropanoids and other natural products derived from amino acids); Biochemistry: Biosynthesis of polypeptides and proteins; structure and function of enzyme and co-enzyme; modeling on bio-organic molecules.

Unit-7: ***Synthetic methodologies with special emphasis on green techniques:*** Introduction to green chemistry; basic principle of green chemistry; green chemistry in day to day life; designing a green synthesis (green reagents, green catalysts, microwave induced green synthesis; ultrasound assisted synthesis; aqueous phase synthesis; solid supported synthesis; synthesis in ionic liquids (global developments in green chemistry and industrial application, pollution prevention; future challenges and perspectives of green chemistry.

Unit-8: ***Asymmetric Synthesis:*** Introduction, kinetic and thermodynamic principles to asymmetric synthesis, diastereoselective & enantioselective synthesis; *Methods of asymmetric synthesis:* Resolution, use of chiral pool, chiral auxiliaries, use of stoichiometric chiral reagents, asymmetric catalysis. Asymmetric hydrogenation, asymmetric reduction of prochiral ketones, asymmetric epoxidation, asymmetric diethylzinc addition to carbonyl compounds, asymmetric aldol reactions (Felkin-anh model), asymmetric Michael reaction. Asymmetric catalysis in water/aqueous media. Applications of L-Proline, (R)- and (S)-BINOL, (+)-Tartaric acid as chiral inducer.

Unit-9: ***Quantum Chemistry:*** The tools of computational chemistry; Concepts of potential energy surface; Ab initio calculations; basic principles of ab initio method, basis sets, post Hartree-Fock calculations, application of ab initio methods; Semi empirical Calculations; DFT, basic principles and applications. WKB approximation and its applications; Scattering theory, Dirac's theory.

Unit-10: ***Spectroscopy and Photochemistry:*** Application of Fluorescence spectroscopy in important photophysical problems; charge transfer, energy transfer, photoisomerization, solvation dynamics, application in Biology and Material Sciences; Ultrafast Spectroscopy: theory and instrumentation, TCSPC, pump probe (flash photolysis, transient absorption), fluorescence upconversion spectroscopy, and application of ultrafast spectroscopy in real-time observation of molecular events; Principle of Lasers; pulsed lasers, Q-switching, cavity dampir g and mode-locking development, applications of pico and femtosecond lasers.

Unit-11: ***Statistical Mechanics:*** Microscopic description of rate theory; Brownian motion; Langevin equation, time correlation functions, correlation functions and Brownian motion, generalization of Langevin equation, Brownian motion in a Harmonic oscillator heat bath, Liouville equation in classical mechanics, generalized Fokker-Planck description of Brownian particles (Van Kampen's approach, Zwanzig's approach), T.S theory, the Kramer's problem and First passage times, overdamped dynamics, application

of Kramer's theory to barrier crossing dynamics, types of noise (white, colored, additive, multiplicative, Levy's, dichotomous).

Unit-12: ***Advanced Electrochemistry:*** Surface Electrochemical Reactivity: the electric double layer, theory of adsorption (Temkin, Fumkin, Anderson-Newns), outer sphere electron transfer (Mercus -Hush theory); Application of Quantum Chemistry and DFT to Surfaces and Interfaces: tunneling effect, electron and proton tunneling at the electrode-electrolyte interface, applications of DFT to electrode-electrolyte interface; Synthesis and Characterization of Electrocatalysts and Nanocatalysts: chemical and electrochemical synthesis, cyclic voltammetry for reversible, quasi reversible and irreversible electrode reactions, SEM, EDX, XRD for characterization of electrocatalysts, single crystal electrodes and their activities at different planes; Fuel cells and Oxygen reduction reactions: alcohol fuel cells, biofuel cells, mediator and mediator less biofuel cells, enzyme immobilization techniques, oxygen reduction and proton exchange membranes.

Unit-13: ***Mathematical Topics:*** Laplace transform; Fourier transform; Dirac delta function; Green's function; Vector algebra and vector calculus; Theory of Polynomials: Legendre and Associated Legendre, Bessel and modified Bessel, Hypergeometric and confluent hypergeometric, Hermite, Lauguerre and Associated Lauguerre.

- Allocation of particular Unit/Units will depend upon its/their availability in that session concerned.