

Chemistry

Ph.D. Course work

Syllabus

Course 1: Research Methodology

4 Credit (60 L)

(Including quantitative methods, Computer Applications, research ethics, review of public research in relevant field, training, field work etc.)

Literature Survey: Print: Sources of information: Primary, secondary, tertiary sources; Journals: Journal abbreviations, abstracts, current titles, reviews, monographs, dictionaries, text-books, current contents, Introduction to Chemical Abstracts and Beilstein, Subject Index, Substance Index, Author Index, Formula Index, and other Indices with examples. Digital: Web resources, E-journals, Journal access, TOC alerts, Hot articles, Citation index, Impact factor, H-index, E-consortium, UGC infonet, E-books, Internet discussion groups and communities, Blogs, Preprint servers, Search engines, Scirus, Google Scholar, ChemIndustry, Wiki- Databases, ChemSpider, Science Direct, SciFinder, Scopus. Information Technology and Library Resources: The Internet and World Wide Web. Internet resources for chemistry. Finding and citing published information

(15 Lectures)

Methods of Scientific Research and Writing Scientific Papers: Reporting practical and project work. Writing literature surveys and reviews. Organizing a poster display. Giving an oral presentation. Writing scientific papers – justification for scientific contributions, bibliography, description of methods, conclusions, the need for illustration, style, publications of scientific work. Writing ethics. Avoiding plagiarism

(15 Lectures)

Chemical Safety and Ethical Handling of Chemicals:

Safe working procedure and protective environment, protective apparel, emergency procedure and first aid, laboratory ventilation. Safe storage and use of hazardous chemicals, procedure for working with substances that pose hazards, flammable or explosive hazards, procedures for working with gases at pressures above or below atmospheric – safe storage and disposal of waste chemicals, recovery, recycling and reuse of laboratory chemicals, procedure for laboratory disposal of explosives, identification, verification and segregation of laboratory waste, disposal of chemicals in the sanitary sewer system, incineration and transportation of hazardous chemicals.

(15 Lectures)

Data Analysis:

The Investigative Approach: Making and Recording Measurements. SI Units and their uses, Scientific method and design of experiments, Analysis and Presentation of Data: Descriptive statistics. Choosing and using statistical tests. Chemometrics. Analysis of variance (ANOVA), Correlation and regression, Curve fitting, fitting of linear equations, simple linear cases, weighted linear case, analysis of residuals, General polynomial fitting, linearizing

transformations, exponential function fit, r and its abuse, basic aspects of the multiple linear regression analysis.

(15 Lectures)

Course 2 :

4 Credit (60 L)

Writing Research Proposal for obtaining financial assistance form

National Funding Agencies 1 credit

Review writing 1 credit

Seminars 2 credit

Subject specific advanced level courses

(Two courses 4 credit each)

Course 3: Instrumental Analysis (Compulsory)

4 Credit (60 L)

Introduction to spectroscopic methods of analysis:

Recap of the spectroscopic methods covered in detail in the core chemistry syllabus: Treatment of analytical data, including error analysis. Classification of analytical methods and the types of instrumental methods. Consideration of electromagnetic radiation.

(04 Lectures)

Molecular spectroscopy:

i) Infrared Spectroscopy:

Interactions with molecules: absorption and scattering. Means of excitation (light sources), separation of spectrum (wavelength dispersion, time resolution), detection of the signal (heat, differential detection), interpretation of spectrum (qualitative, mixtures, resolution), advantages of Fourier Transform (FTIR). Samples and results expected. Applications: Issues of quality assurance and quality control, Special problems for portable instrumentation and rapid detection.

(08 Lectures)

ii) UV-Visible/ Near IR – emission, absorption, fluorescence and photoacoustic. Excitation sources (lasers, time resolution), wavelength dispersion (gratings, prisms, interference filters, laser, placement of sample relative to dispersion, resolution), Detection of signal (photocells, photomultipliers, diode arrays, sensitivity and S/N), Single and Double Beam instruments, Interpretation (quantification, mixtures, absorption vs. fluorescence and the use of time, photoacoustic, fluorescent tags).

(08 Lectures)

iii) Separation techniques

Chromatography: Gas chromatography, liquid chromatography, supercritical fluids, Importance of column technology (packing, capillaries), Separation based on increasing number of factors (volatility, solubility, interactions with stationary phase, size, electrical field), Detection: simple vs. specific (gas and liquid), Detection as a means of further analysis

(use of tags and coupling to IR and MS), Electrophoresis (plates and capillary) and use with DNA analysis. Immunoassays and DNA techniques **(08 Lectures)**

iv) Mass spectroscopy: Making the gaseous molecule into an ion (electron impact, chemical ionization), Making liquids and solids into ions (electrospray, electrical discharge, laser desorption, fast atom bombardment), Separation of ions on basis of mass to charge ratio, Magnetic, Time of flight, Electric quadrupole. Resolution, time and multiple separations, Detection and interpretation (how this is linked to excitation). **(10 Lectures)**

iv) Atomic spectroscopy: Atomic absorption, Atomic emission, and Atomic fluorescence. Excitation and getting sample into gas phase (flames, electrical discharges, plasmas), Wavelength separation and resolution (dependence on technique), Detection of radiation (simultaneous/scanning, signal noise), Interpretation (errors due to molecular and ionic species, matrix effects, other interferences). **(06 Lectures)**

NMR spectroscopy: Principle, Instrumentation, Factors affecting chemical shift, Spincoupling, Applications.

(4 Lectures)

Electroanalytical Methods: Potentiometry & Voltammetry

(4 Lectures)

Radiochemical Methods

(4 Lectures)

X-ray analysis and electron spectroscopy (surface analysis)

(4 Lectures)

Reference books:

- D.A. Skoog, F.J. Holler & S. Crouch (ISBN 0-495-01201-7) Principles of Instrumental
- Analysis, Cengage Learning India Edition, 2007.
- Willard, Merritt, Dean, Settle, Instrumental Methods of Analysis, 7th ed, IBH Book
- House, New Delhi.
- Atkins, P.W & Paula, J.D. Physical Chemistry, 10th Ed., Oxford University Press (2014).
- Kakkar, R. Atomic and Molecular Spectroscopy: Concepts and Applications. Cambridge
- University Press, 2015.
- Castellan, G. W. Physical Chemistry 4th Ed., Narosa (2004).
- Banwell, C. N. & McCash, E. M. Fundamentals of Molecular Spectroscopy 4th Ed. Tata McGrawHill: New Delhi (2006).

Course 4 : Any TWO form the following (Each part is of 2 Credit)

Part I : NANOMATERIALS: (02 Credit , 30 L)

The Big world of nanomaterials

History and scope-Can small things make big difference? – Classification of nanomaterials – Fascinating Nanostructures –Applications of nanomaterials- The nature: The Bets Nanotechnologist – Challenges and future prospects

Unique Properties of Nanomaterials

Microstructure and defects in monocrystalline Materials-Effect of Nano dimensions on material behaviour

Optical Properties ,Electrical Properties , Mechanical Properties, Magnetic Properties

Synthesis Routes

Bottom-Up approaches – Top-Down approaches- Consolidation of Nano powders Mechanical Grinding, Wet Chemical Synthesis of Nanomaterials –Sol Gel Process, Gas Phase Synthesis, Flame assisted ultrasonic spray pyrolysis, Gas Condensation Processing, Chemical Vapour Condensation (CVC) etc.

Application of Nanomaterials

Nano electronics –Micro and Nano-Electromechanical Systems (MEMS/NEMS) – Nanosensors –Nanocatalysts- Food and Agriculture Industries – Cosmetic and Consumer goods – Structure and Engineering – Automotive Industry-Water treatment and environment – Nanomedical applications – Textile-Paints –Energy-Defence and space applications – Structural applications , etc.

Tools to Characterize Nanomaterials

X-Ray Diffraction (XRD) – Small Angle X Ray Scattering (SAXS)-Scanning Electron microscopy (SEM) – Transmission Electron Microscope (TEM)-Atomic Force Microscope (AFM) –Scanning Tunnelling Microscope (STM) - Field Ion Microscope (FIM) –Three Dimensional Atom Probe (3DAP) –Nano indentation

Concern and Challenges of Nanotechnology

References

1. Text Book of Nanoscience and Nanotechnology by B S Murty , P Shankar , Baldev Raj, B B Rath, James Murday – Springer and University Press (2013)
2. Chapter - Introduction to Nanomaterial - Alagarasi, A, -2016-Research Gate

Fundamentals: mathematical functions, polynomial expressions, logarithms, the exponential function, units of a measurement, interconversion of units, constants and variables, equation of a straight line, plotting graphs.

Uncertainty in experimental techniques: Displaying uncertainties, measurements in chemistry, decimal places, significant figures, combining quantities.

Uncertainty in measurement: types of uncertainties, combining uncertainties. Statistical treatment. Mean, standard deviation, relative error. Data reduction and the propagation of errors. Graphical and numerical data reduction. Numerical curve fitting: the method of least squares (regression).

Algebraic operations on real scalar variables (e.g. manipulation of van der Waals equation in different forms). Roots of quadratic equations analytically and iteratively (e.g. pH of a weak acid). Numerical methods of finding roots (Newton-Raphson, binary –bisection, e.g. pH of a weak acid not ignoring the ionization of water, volume of a van der Waals gas, equilibrium constant expressions).

Differential calculus: The tangent line and the derivative of a function, numerical differentiation (e.g., change in pressure for small change in volume of a van der Waals gas, potentiometric titrations).

Numerical integration (Trapezoidal and Simpson's rule, e.g. entropy/enthalpy change from heat capacity data).

Computer programming:

Constants, variables, bits, bytes, binary and ASCII formats, arithmetic expressions, hierarchy of operations, inbuilt functions. Elements of the BASIC language. BASIC keywords and commands. Logical and relative operators. Strings and graphics. Compiled versus interpreted languages. Debugging. Simple programs using these concepts. Matrix addition and multiplication. Statistical analysis. BASIC programs for curve fitting, numerical differentiation and integration (Trapezoidal rule, Simpson's rule), finding roots (quadratic formula, iterative, Newton-Raphson method).

Numeric modelling: Simulation of pH metric titration curves. Excel functions LINEST and Least Squares. Numerical curve fitting, linear regression (rate constants from concentrationtime data, molar extinction coefficients from absorbance data), numerical differentiation (e.g. handling data from potentiometric and pH metric titrations, pKa of weak acid), integration (e.g. entropy/enthalpy change from heat capacity data). Statistical analysis: Gaussian distribution and Errors in measurements and their effect on data sets. Descriptive statistics using Excel. Statistical significance testing: The t test. The F test.

Presentation: Presentation graphics

Additional Work :

HANDS ON ACTIVITY

Introductory writing activities: Introduction to word processor and structure drawing (ChemSketch) software. Incorporating chemical structures, chemical equations, expressions from chemistry (e.g. Maxwell-Boltzmann distribution law, Bragg's law, van der Waals equation, etc.) into word processing documents.

Handling numeric data: Spreadsheet software (Excel), creating a spreadsheet, entering and formatting information, basic functions and formulae, creating charts, tables and graphs.

Incorporating tables and graphs into word processing documents. Simple calculations, plotting graphs using a spreadsheet (Planck's distribution law, radial distribution curves for

hydrogenic orbitals, gas kinetic theory- Maxwell-Boltzmann distribution curves as function of temperature and molecular weight), spectral data, pressure-volume curves of van der Waals gas (van der Waals isotherms), data from phase equilibria studies. Graphical solution of equations.

Reference Books:

- McQuarrie, D. A. Mathematics for Physical Chemistry University Science Books (2008).
- Mortimer, R. Mathematics for Physical Chemistry. 3rd Ed. Elsevier (2005).
- Steiner, E. The Chemical Maths Book Oxford University Press (1996).
- Yates, P. Chemical calculations. 2nd Ed. CRC Press (2007).
- Harris, D. C. Quantitative Chemical Analysis. 6th Ed., Freeman (2007) Chapters 3-5.
- Levie, R. de, How to use Excel in analytical chemistry and in general scientific data analysis, Cambridge Univ. Press (2001) 487 pages.
- Noggle, J. H. Physical chemistry on a Microcomputer. Little Brown & Co. (1985).
- Venit, S.M. Programming in BASIC: Problem solving with structure and style. Jaico Publishing House: Delhi (1996)

Part III : CHEMICAL TECHNOLOGY & SOCIETY (30 L 2 Credit)

Chemical Technology

Basic principles of distillation, solvent extraction, solid-liquid leaching and liquid-liquid extraction, separation by absorption and adsorption. An introduction into the scope of different types of equipment needed in chemical technology, including reactors, distillation, extruders, pumps, mills, emulgators. Scaling up operations in chemical industry. Introduction to clean technology.

Society

Exploration of societal and technological issues from a chemical perspective. Chemical and scientific literacy as a means to better understand topics like air and water (and the trace materials found in them that are referred to as pollutants); energy from natural sources (i.e. solar and renewable forms), from fossil fuels and from nuclear fission; materials like plastics and polymers and their natural analogues, proteins and nucleic acids, and molecular reactivity and interconversions from simple examples like combustion to complex instances like genetic engineering and the manufacture of drugs.

Reference Book:

- John W. Hill, Terry W. McCreary & Doris K. Kolb, Chemistry for changing times 13th Ed, Prentice-Hall (2012).

Part IV : ANALYTICAL CLINICAL BIOCHEMISTRY

(30 L 2 Credit)

Basic understanding of the structures, properties and functions of carbohydrates, lipids and proteins: Review of concepts studied in the core course:

Carbohydrates: Biological importance of carbohydrates, Metabolism, Cellular currency of energy (ATP), Glycolysis, Alcoholic and Lactic acid fermentations, Krebs cycle.

Isolation and characterization of polysaccharides.

Proteins: Classification, biological importance; Primary and secondary and tertiary structures of proteins: α -helix and β -pleated sheets, Isolation, characterization, denaturation of proteins.

Enzymes: Nomenclature, Characteristics (mention of Ribozymes), Classification; Active site, Mechanism of enzyme action, Stereospecificity of enzymes, Coenzymes and cofactors,

Enzyme inhibitors, Introduction to Biocatalysis: Importance in “Green Chemistry” and Chemical Industry.

Lipids: Classification. Biological importance of triglycerides and phosphoglycerides and cholesterol; Lipid membrane, Liposomes and their biological functions and underlying applications. Lipoproteins. Properties, functions and biochemical functions of steroid hormones.

Biochemistry of peptide hormones.

Structure of DNA (Watson-Crick model) and RNA, Genetic Code, Biological roles of DNA and RNA: Replication, Transcription and Translation, Introduction to Gene therapy.

Enzymes: Nomenclature, classification, effect of pH, temperature on enzyme activity, enzyme

inhibition.

Biochemistry of disease: A diagnostic approach by blood/ urine analysis.

Blood: Composition and functions of blood, blood coagulation. Blood collection and preservation of samples. Anaemia, Regulation, estimation and interpretation of data for blood sugar, urea, creatinine, cholesterol and bilirubin.

Urine: Collection and preservation of samples. Formation of urine. Composition and estimation of constituents of normal and pathological urine.

Reference Books:

- Cooper, T.G. Tool of Biochemistry. Wiley-Blackwell (1977).
- Wilson, K. & Walker, J. Practical Biochemistry. Cambridge University Press (2009).
- Varley, H., Gowenlock, A.H & Bell, M.: Practical Clinical Biochemistry, Heinemann, London (1980).
- Devlin, T.M., Textbook of Biochemistry with Clinical Correlations, John Wiley & Sons, 2010.
- Berg, J.M., Tymoczko, J.L. & Stryer, L. Biochemistry, W.H. Freeman, 2002.

- Talwar, G.P. & Srivastava, M. Textbook of Biochemistry and Human Biology, 3rd Ed.
- PHI Learning.
- Nelson, D.L. & Cox, M.M. Lehninger Principles of Biochemistry, W.H. Freeman, 2013.
- O. Mikes, R.A. Chalmers: Laboratory Handbook of Chromatographic Methods, D. Van Nostrand & Co., 1961.

Part V : GREEN CHEMISTRY

(02 Credits , 30 L)

Introduction : Brief introduction of twelve principles of Green Chemistry, with examples, special emphasis on atom economy, reducing toxicity, green solvents, Green Chemistry and catalysis and alternative sources of energy, Green energy and sustainability

The following Real world Cases in Green Chemistry should be discussed:

- Surfactants for carbon dioxide – Replacing smog producing and ozone depleting solvents with CO₂ for precision cleaning and dry cleaning of garments.
- Designing of environmentally safe marine antifoulant.
- Rightfit pigment: Synthetic azo pigments to replace toxic organic and inorganic pigments.
- An efficient, green synthesis of a compostable and widely applicable plastic (poly lactic acid) made from corn. copper(II).

Reference Books:

- Anastas, P.T. & Warner, J.K. Green Chemistry- Theory and Practical, Oxford University Press (1998).
- Matlack, A.S. Introduction to Green Chemistry, Marcel Dekker (2001).
- Cann, M.C. & Connely, M.E. Real-World cases in Green Chemistry, American Chemical Society, Washington (2000).
- Ryan, M.A. & Tinnesand, M. Introduction to Green Chemistry, American Chemical Society, Washington (2002).
- Sharma, R.K.; Sidhwani, I.T. & Chaudhari, M.K. Green Chemistry Experiments: A monograph I.K. International Publishing House Pvt Ltd. New Delhi, Bangalore.
- Lancaster, M. Green Chemistry: An introductory text RSC publishing, 2nd Edition.
- Sidhwani, I.T., Saini, G., Chowdhury, S., Garg, D., Malovika, Garg, N. Wealth from waste: A green method to produce biodiesel from waste cooking oil and generation of useful products from waste further generated “A Social Awareness Project”, Delhi University Journal of Undergraduate Research and Innovation, 1(1): 2015.

Part VI : PHARMACEUTICAL CHEMISTRY

(30 L 2 Credit)

Drugs & Pharmaceuticals

Drug discovery, design and development; Basic Retrosynthetic approach. Synthesis of the representative drugs of the following classes: analgesics agents, antipyretic agents, antiinflammatory agents (Aspirin, paracetamol, Ibuprofen); antibiotics (Chloramphenicol);

antibacterial and antifungal agents (Sulphonamides; Sulphanethoxazol, Sulphacetamide, Trimethoprim); antiviral agents (Acyclovir), Central Nervous System agents (Phenobarbital, Diazepam), Cardiovascular (Glyceryl trinitrate), antilaprosy (Dapsone), HIV-AIDS related drugs (AZT- Zidovudine).

Fermentation

Aerobic and anaerobic fermentation. Production of (i) Ethyl alcohol and citric acid, (ii) Antibiotics; Penicillin, Cephalosporin, Chloromycetin and Streptomycin, (iii) Lysine, Glutamic acid, Vitamin B2, Vitamin B12 and Vitamin C

Reference Books:

- Patrick, G. L. Introduction to Medicinal Chemistry, Oxford University Press, UK, 2013.
- Singh, H. & Kapoor, V.K. Medicinal and Pharmaceutical Chemistry, Vallabh Prakashan, Pitampura, New Delhi, 2012.
- Foye, W.O., Lemke, T.L. & William, D.A.: Principles of Medicinal Chemistry, 4th ed., B.I. Waverly Pvt. Ltd. New Delhi

Part VII : FUEL CHEMISTRY

(30 L 2 Credit)

Review of energy sources (renewable and non-renewable). Classification of fuels and their calorific value.

Coal: Uses of coal (fuel and nonfuel) in various industries, its composition, carbonization of coal. Coal gas, producer gas and water gas—composition and uses. Fractionation of coal tar, uses of coal tar bases chemicals, requisites of a good metallurgical coke, Coal gasification (Hydro gasification and Catalytic gasification), Coal liquefaction and Solvent Refining.

Petroleum and Petrochemical Industry: Composition of crude petroleum, Refining and different types of petroleum products and their applications. Fractional Distillation (Principle and process), Cracking (Thermal and catalytic cracking), Reforming Petroleum and non-petroleum fuels (LPG, CNG, LNG, bio-gas, fuels derived from biomass), fuel from waste, synthetic fuels (gaseous and liquids), clean fuels.

Petrochemicals: Vinyl acetate, Propylene oxide, Isoprene, Butadiene, Toluene and its derivatives Xylene.

Lubricants: Classification of lubricants, lubricating oils (conducting and non-conducting) Solid and semisolid lubricants, synthetic lubricants. Properties of lubricants (viscosity index, cloud point, pore point) and their determination.

Reference Books:

- Stocchi, E. Industrial Chemistry, Vol-I, Ellis Horwood Ltd. UK (1990).
- Jain, P.C. & Jain, M. Engineering Chemistry Dhanpat Rai & Sons, Delhi.
- Sharma, B.K. & Gaur, H. Industrial Chemistry, Goel Publishing House, Meerut (1996).

Part VIII : INORGANIC MATERIALS

(30 L 2 Credit)

Glass: Glassy state and its properties, classification (silicate and non-silicate glasses). Manufacture and processing of glass. Composition and properties of the following types of glasses: Soda lime glass, lead glass, armoured glass, safety glass, borosilicate glass, fluorosilicate, coloured glass, photosensitive glass.

Ceramics: Important clays and feldspar, ceramic, their types and manufacture. High technology ceramics and their applications, superconducting and semiconducting oxides, fullerenes carbon nanotubes and carbon fibre.

Surface Coatings:

Objectives of coatings surfaces, preliminary treatment of surface, classification of surface coatings. Paints and pigments-formulation, composition and related properties. Oil paint, Vehicle, modified oils, Pigments, toners and lakes pigments, Fillers, Thinners, Enamels, emulsifying agents. Special paints (Heat retardant, Fire retardant, Eco-friendly paint, Plastic paint), Dyes, Wax polishing, Water and Oil paints, additives, Metallic coatings (electrolytic and electroless), metal spraying and anodizing.

Batteries:

Primary and secondary batteries, battery components and their role, Characteristics of Battery. Working of following batteries: Pb acid, Li-Battery, Solid state electrolyte battery. Fuel cells, Solar cell and polymer cell.

Chemical explosives:

Origin of explosive properties in organic compounds, preparation and explosive properties of lead azide, PETN, cyclonite (RDX). Introduction to rocket propellants.

Reference Books:

- E. Stocchi: Industrial Chemistry, Vol-I, Ellis Horwood Ltd. UK.
 - R. M. Felder, R. W. Rousseau: Elementary Principles of Chemical Processes, Wiley Publishers, New Delhi.
 - W. D. Kingery, H. K. Bowen, D. R. Uhlmann: Introduction to Ceramics, Wiley Publishers, New Delhi.
 - J. A. Kent: Riegel's Handbook of Industrial Chemistry, CBS Publishers, New Delhi.
 - P. C. Jain, M. Jain: Engineering Chemistry, Dhanpat Rai & Sons, Delhi.
 - R. Gopalan, D. Venkappayya, S. Nagarajan: Engineering Chemistry, Vikas Publications, New Delhi.
 - Sharma, B.K. & Gaur, H. Industrial Chemistry, Goel Publishing House, Meerut (1996).
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