

Syllabus
Of
Pre-Ph.D. Course Work
In
Chemistry

Department of
Applied Sciences & Humanities
Invertis Institute of Engineering & Technol.
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Bareilly-Lucknow NH-24, Bareilly-243123, India

PhDCY 191: *Computer Fundamentals and Numerical Analysis*

Fundamentals of computers

Computer fundamentals, hardwares and softwares, different operating systems, application programmes, some tips on PC maintenance and servicing of PC.

Common Applications: Working in a Linux environment, basic Linux commands, writing scientific documents with Latex, graphic and visualization, gnuplot; introduction to other useful software tools e.g. mathematica

Basic Numerical Methods: Numerical integration (trapezoidal and Simpson's method), numerical differentiation; Diagonalization and inverse of symmetric and non-symmetric matrices, Eigenvalues and eigenvectors.; Root finding (bisection and Newton-Raphson method); Interpolation techniques; Solution of ordinary differential equations (Euler and Runge-Kutta methods).

Statistics and treatment of experimental data: Data acquisition system, error propagation, curve fitting, Least square method, Sampling and parameter estimation, the maximum likelihood method. Analysis of a time series and search for periodicity. FFT (Fast Fourier transformation) and power spectrum and any other topics used in physics researches.

Simulation and Monte Carlo Method: Simulation of Random variables, discrete and continuous. Calculation of integrals. Monte Carlo evaluation of pi. Simulation of simple processes: coin tossing or dice throwing game. Examples and applications.

Reference Books :

1. *Numerical methods for Scientific and Engineering Computation: M.K.Jain, S.R.K.Iyengar and R.K.Jain. (Wiley Eastern Limited),*
2. *Techniques for Nuclear and Particle Physics Experiments, A How to approach: W.R.Leo (Narosa Publishing House)*
3. *Numerical Recipes: W.Press et.al., (Cambridge University Press).* 4. *Data reduction and error analysis for the Physical Sciences, 3e, Philip R*

(PhDCY-102) GENERAL CHEMISTRY

Colloids:

Colloids, the colloidal state, preparation and purification of colloids and their characteristic properties, lyophilic and lyophobic colloids and coagulation, protection of colloids, gels, emulsions, surfactants and micelles.

Surface phenomenon

Surface tension of liquids-capillary action, experimental determination of surface tension, temperature effect on surface tension. Viscosity of liquids, experimental determination of viscosity coefficient, its variation with temperature.

Kinetic theory of gases, ideal gas laws based on kinetic theory. Collision in a gas-mean free path, collision diameter, collision number. Behaviour of real gases-the van der Waal's equation. Critical phenomena-critical constants of a gas and their determination.

Hardness:

Chemistry of Hydrogen, Hydrogen peroxide including manufacturing and structure, Heavy

Hydrogen, Heavy water, ortho and Para Hydrogen. Hardness of water, removal & estimation of hardness

Organic Compounds:

Classification, and Nomenclature, Hybridization, Shapes of molecules.

Electronic Displacements: Inductive, Electromeric, Resonance effects and Hyperconjugation. Homolytic and Heterolytic fission. Electrophiles and Nucleophiles. Types, shape and relative stability of intermediates (Carbocations, Carbanions, Free radicals and Carbenes). Introduction of organic reactions : Addition, Elimination and Substitution reactions.

Recommended Books:

1. B. R. Puri, L. R. Sharma, and M. S. Pathania. 37th Edition (1998), Shoban Lal Nagin Chand & Co., Jalandhar.
2. P. Atkins and J. De Paul, 8th Edition (2006), International Student Edition, Oxford University Press.
3. I. L. Finar, Vol. I, 6th Edition (1973), ELBS and Longman Ltd., New Delhi.

PhDCY 103(3 to 11) Chemistry: OPTIONAL

Note: Student has to choose one of the following papers. There is provision to add more optional papers subject to the availability of manpower in concerned field.

1. Surfactants (PhDCY-103)
2. Conducting polymers (PhDCY-104)
3. Coordination chemistry (PhDCY-105)
4. Thermodynamics(PhDCY-106)
5. Chemistry of natural products. (PhDCY-107)
6. polymers(PhDCY-108)
7. Electrochemistry(PhDCY-109)
8. Chemical kinetics(PhDCY-110)
9. Heterocyclic Compounds (PhDCY-111)

Surfactants (PhDCY-103)

Surfactants and their classifications; Surface and interfacial tensions and free energies; Colloidal interactions in water; Colloidal stability; Adsorption and adhesion. Kinetics of adhesion/adsorption; Surface properties of clays and other minerals; Biosurfaces; Association colloids formed by surfactants: micelles, bilayers, microemulsions, surfactant phase behavior; Detergency & emulsions; Polymer structure and properties in solid state & solution; Applications of surfactants and polymers in paints & coatings; Characterization of colloids and surfaces; Colloid & surface phenomena in product design; Nanotechnology. enhanced oil recovery

Books:

1. W. Adamson & A. P. Gast: "Physical Chemistry of Surfaces", 6th ed., Wiley, 1997.
2. J. N. Israelachvili: "Intermolecular and Surface Forces", 2nd ed., Academic Press, 1992.
3. P. C. Hiemenz & R. Rajagopalan: "Principles of Colloid and Surface Chemistry", 3rd ed., Marcel Dekker, 1997.

Conducting polymers (PhDCY 104)

electrochemistry of electronically conducting polymers-source of electronic conduction in polymers – solitons , polarons and bipolarons – emiconductors and conducting polymers. Synthesis of conducting polymers – chemical, electrochemical and enzymatic methods –doping –general considerations – measurement of conductivity – van der Pauw technique –factors affecting conductivity.

Characterization of conducting polymers – electroanalytical techniques – cyclic voltammetry, chronoamperometry and chronocoulometry, spectral methods - use of UVvis,Raman, XRD and NMR.

Synthesis, processability and applications of acetylene, aniline, pyrrole, thiophene and para– phenylene based conducting polymers.

Conducting polymers in microelectronics – corrosion and ESD protection, EMI shielding and lithography. LED-rechargeable batteries – artificial muscles - electrochromic devices–sensor devices–conductive composites.

Books -

- 1.T.A. Skotheim, R.L. Elsenbaumer and J.R. Reynolds, Hand book of Conducting Polymers - 2nd Edn, Revised and enlarged, Marcel Dekker, Inc., New York, 1998.
2. J.M. Margolis (Ed.), Conducting Polymers and Plastics, Chapman and Hall, London,1989.
3. R.B. Seymour, ed., Conductive Polymers”, Plenum Press, New York, 1981.

Coordination chemistry (PhDCY 105)

Werner's theory, valence bond theory (inner and outer orbital complexes), electroneutrality principle and back bonding. Crystal field theory, measurement of $10 Dq$ (o), CFSE in weak and strong fields, pairing energies, factors effecting the magnitude of $10 Dq$ (o, t). Octahedral vs. tetrahedral coordination, tetragonal distortions from octahedral geometry Jahn-Teller theorem, square planar geometry.

IUPAC nomenclature of coordination compounds, isomerism in coordination compounds. Stereochemistry of complexes with 4 and 6 coordination numbers. Chelate effect, polynuclear complexes.

Books:

1. Purecell, K.F. and Kotz, J.C., *Inorganic Chemistry* W.B. Saunders Co. 1977.
2. Basolo, F, and Pearson, R.C., *Mechanisms of Inorganic Chemistry*, John Wiley & Sons, NY, 1967.

Thermodynamics (PhDCY 106)

First law of thermodynamics and their applications, thermodynamic system, states and processes work, heat and internal energy, zeroth law of thermodynamics, various types of work done on a system in reversible and irreversible process, Calorimetry and thermochemistry, enthalpy changes in various physical and chemical process, second law of thermodynamics and its applications.

Books:

1. Atkins, P. W. & Paula, J. de *Atkin's Physical Chemistry* 8th Ed., Oxford University Press (2006).
2. Castellan, G. W. *Physical Chemistry* 4th Ed. Narosa (2004).
3. Engel, T. & Reid, P. *Thermodynamics, Statistical Thermodynamics, & Kinetics* Pearson Education, Inc: New Delhi (2007).
4. McQuarrie, D. A. & Simon, J. D. *Molecular Thermodynamics* Viva Books Pvt. Ltd.: New Delhi (2004).

Chemistry of natural products. (PhDCY 107)

Alkaloids: Structure elucidation of alkaloids – a general account; Structure, synthesis, and stereochemistry of Narcotine and Quinine; synthesis and stereochemistry of Morphine, Lysergic acid and Reserpine.

Terpenoids: Camphor, Longifolene*, Abietic acid, and Taxol.

Steroids: Cholesterol, Cortisone*, and Aldosterone*.

Prostaglandins and Thromboxanes : Introduction, nomenclature of prostaglandins and thromboxanes; approaches to prostaglandin synthesis; cyclohexane precursors (Woodward synthesis of PGF_{2a}), bicycloheptane precursors (Corey's synthesis of prostaglandins E and F)

Books:

1. Nitya Anand, J.S. Bindra and S. Ranganathan, *Art in Organic Synthesis*, 2nd Edition (1970), Holden Day, San Francisco.
2. S.W. Pelletier, *Chemistry of the Alkaloids*, Van Nostrand Reinhold Co., New York (1970).
3. K.W. Bentley, *The Alkaloids*, Vol. I., Interscience Publishers, New York (1957).
4. I. L. Finar, *Organic Chemistry*, Vol. II, 5th Edition (1975) Reprinted in 1996, ELBS and Longman Ltd, New Delhi
5. J.W. Apsimon, *Total Synthesis of Natural Products*, Vol. 1-6, Wiley-Interscience Publications, New York.

Polymers (PhDCY 108)

Introduction and classification polymers; Number average molecular weight, Weight average molecular weight, Degree of polymerization, Polydispersity Index.

Polymerisation reactions - Addition and condensation - Mechanism of cationic, anionic and free radical addition polymerization. Preparation and applications of plastics – thermosetting (phenol-formaldehyde) and thermosoftening (PVC, polythene); Rubbers – natural and synthetic: Buna-S, Chloroprene and Neoprene; Vulcanization; Biodegradable and conducting polymers with examples

Books:

1. Kemp, W. *Organic Spectroscopy*, Palgrave.
2. Kalsi, P. S. *Textbook of Organic Chemistry* (1st Ed.), New Age International (P) Ltd.
3. Morrison, R. T. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
4. Billmeyer, F. W. *Textbook of Polymer Science*, John Wiley & Sons, Inc.
5. Gowariker, V. R., Viswanathan, N. V. & Sreedhar, J. *Polymer Science*, New Age International (P) Ltd. Pub

Electrochemistry (PhDCY 109)

Quantitative aspects of Faraday's laws of electrolysis, rules of oxidation/reduction of ions based on half-cell potentials, applications of electrolysis in metallurgy and industry. Chemical cells, reversible and irreversible cells with examples. Electromotive force of a cell and its measurement, Nernst equation; Standard electrode (reduction) potential and its application to different kinds of half-cells. Application of EMF measurements in determining (i) free energy, enthalpy and entropy of a cell reaction, (ii) equilibrium constants, and (iii) pH values, using hydrogen, quinone-hydroquinone, glass and $\text{SbO/Sb}_2\text{O}_3$ electrodes. Concentration cells with and without transference, liquid junction potential; determination of activity coefficients and transference numbers. Qualitative discussion of potentiometric titrations (acid-base, redox, precipitation, Arrhenius theory of electrolytic dissociation, Hydrolysis of salts, hydrolysis constant, buffer solutions, indicators and theory of acid-base indicators.

Books:

1. Atkins, P. W. & Paula, J. de *Atkin's Physical Chemistry* 8th Ed., Oxford University Press (2006).
2. Castellan, G. W. *Physical Chemistry* 4th Ed. Narosa (2004).
3. Engel, T. & Reid, P. *Thermodynamics, Statistical Thermodynamics, & Kinetics* Pearson Education, Inc: New Delhi (2007).

Chemical kinetics (PhDCY 110)

Order and molecularity of a reaction, rate laws in terms of the advancement of a reaction,

differential and integrated form of rate expressions up to second order reactions, experimental

methods of the determination of rate laws, kinetics of complex reactions (integrated rate expressions up to first order only): (i) Opposing reactions (ii) parallel reactions and (iii) chain reactions.

Temperature dependence of reaction rates; Arrhenius equation; activation energy.

Collision theory of reaction rates. Surface chemistry: Physical adsorption, chemisorption, adsorption isotherms. nature of adsorbed state.

Catalysis: Types of catalyst, specificity and selectivity, mechanisms of catalyzed reactions at solid surfaces; effect of particle size and efficiency of nanoparticles as catalysts.

Books:

1. Atkins, P. W. & Paula, J. de *Atkin's Physical Chemistry* 8th Ed., Oxford University Press (2006).
2. Ball, D. W. *Physical Chemistry* Thomson Press, India (2007).
3. Castellan, G. W. *Physical Chemistry* 4th Ed. Narosa (2004).
4. Laidler, K. J. *Chemical Kinetics* Pearson Education: New Delhi (2004).

Heterocyclic Compounds (PhDCY 111)

Classification and nomenclature, Structure, aromaticity in 5-numbered and 6-membered rings containing one heteroatom; Synthesis, reactions and mechanism of substitution reactions of: Furan, Pyrrole (Paal-Knorr synthesis, Knorr pyrrole synthesis, Hantzsch synthesis), Thiophene, Pyridine (Hantzsch synthesis), Pyrimidine, Structure elucidation of indole, Fischer indole synthesis and Madelung synthesis), Structure elucidation of quinoline and isoquinoline, Skraup synthesis, Friedlander's synthesis, Knorr quinoline synthesis, Doebner-Miller synthesis, Bischler-Napieralski reaction, Pictet-Spengler reaction, Pomeranz-Fritsch reaction, Derivatives of furan: Furfural and furoic acid.

Recommended Texts:

1. Morrison, R. T. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
2. Finar, I. L. *Organic Chemistry (Volume 1)*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
3. Finar, I. L. *Organic Chemistry (Volume 2: Stereochemistry and the Chemistry of Natural Products)*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).