CHOICE BASED CREDIT SYSTEM (CBCS)

Ph. D. Course Work

Syllabus for Chemistry

ABOUT THE DEPARTMENT

Department of Chemistry, IGNTU, Amarkantak

The Department of Chemistry was started in 2008, and has now grown into a major department for teaching and research within the Faculty of Science at IGNTU. The department offer vibrant atmosphere to students and faculty to encourage the spirit of scientific inquiry and to pursue cutting-edge research in a highly encouraging environment. The key objective of our department is to create good quality human resource through competitive yet inspiring environment for developing their careers. Currently, the department comprises more than hundred students, five research scholar and seven faculties and a dedicate team of staff members. The department offers three years undergraduate B.Sc. courses in Chemistry (Hons.) in the University. In addition it also offers two years M. Sc. and PhD programme. At present the Department consists of about seven research groups working in the areas of material chemistry (Functional Hybrid Nanomaterials), coordination/ supramolecular chemistry, bioinorganic chemistry, asymmetric synthesis, catalysis, nanomagnetism and Single Molecule Magnets (SMMs), as major thrust areas. The department is doing well in research activities and published good numbers of research papers. The faculty has been undertaking research projects sponsored by different national agencies such as DST, UGC, etc. The most important achievement of the University is the first Department of Chemistry has succeeded "**DST-FIST Program – 2017**" recognition from Govt. of India, Department of Science & Technology, New Delhi**.** Many students have been qualified National Eligibility Test (NET) and Joint Admission Test (JAM) Examination for pursuing PhD and M. Sc. Program in different prestigious IIT, NIT and Central Universities. The most of the students of our department is tribal and our mission is that the department of Chemistry can be reached at highest level in the country for its teaching and research activities and produced number of best quality of students in India.

At a Glance Department of Chemistry, IGNTU

Faculty Profile

Presentation	Name & Designation	Research Area	Awards and Honors
	**Dr. Tanmay K Ghorai** Associate Professor & Head *PhD: IIT-KGP*	Nanoscience, Catalysis & Single Molecule Magnets	BOYSCAST Fellowship & Young Scientist Award (DST)
	**Dr. Subrata Jana** Associate Professor *PhD: IIEST-Shibpur*	Molecular Recognition & Supramolecular Chemistry	Radhika Panda Memorial Award, UrFU PDF Award
	**Dr. Khemchand Dewangan** Assistant Professor *PhD: IIT-Kanpur*	Nanostructure Transition Metal Oxides & Nitrides	BSR-UGC Start-Up Grant
	**Dr. Adhish Jaiswal** Assistant Professor *PhD: NCL-Pune*	Dieletrics, Magnetism & Solar-cell	Best Research Scholar Award in NCL Pune
	**Dr. Biswajit Maji** Assistant Professor *PhD: IIT-KGP*	Asymmetric Synthesis and Catalysis	INSPIRE Faculty Award, President INSPIRE Teacher Recognition
	**Dr. Sadhu Charan Mallick** Assistant Professor *PhD: IITGuwahati*	Metal Nano Particles, Polymer Composites & Bio applications	Best Poster Award at IICT Hyderabad
	**Dr. Ajay Shankar** Assistant Professor *PhD: NPL, Delhi*	Nano-magnetism	Post- Doctoral fellowship Award at Germany

Members of the Board of Studies

For

Revised the Chemistry Syllabus for

Ph. D. Courses

According

CHOICE BASED CREDIT SYSTEM (CBCS)

The syllabus of Ph.D. (Course Work) is hereby approved in a meeting of the members of the Board of Study for the Department of Chemistry, Indira Gandhi National Tribal University, Amarkantak (M.P.) on February 6, 2017, Monday.

Prof. Ashish K. Prajapati
Professor
(Member, External Expert)
Department of Chemistry,
The M. S. University of Baroda

Dr. Raghumani Singh Ningthoujam
Scientist-E
(Member, Special Invitee)
Chemistry Division
Bhabha Atomic Research Centre

Dr. Tarun Thakur
Associate Professor
(Member)
Department of Environmental Science
IGNTU

Dr. Ravindra Shukla
Assistant Professor
(Member)
Department of Botany
IGNTU

Dr. Subrata Jana
Associate Professor
(Member)
Department of Chemistry
IGNTU

Dr. Tanmay Kumar Ghorai
Associate Professor & Head
(Chairman)
Department of Chemistry
IGNTU

Course Structure for PhD Course Work

CHEMISTRY

The PhD course work course comprises common courses (05 credits; **A**), Research theme - Common Elective Courses (04 credits; **B**) and Discipline Specific Elective Courses (06 Credits; **C**). Since PhD students come from different educational backgrounds, relevant courses will be chosen in consultation with the concerned DRC to compliment the previous education, improve specific skills required for thesis and subsequent career. The *Common Courses* (CHM T 700), for all PhD scholars registered in chemical science related disciplines with the Faculty of Science in the Indira Gandhi National Tribal University, Amarkantak. *Research Them- Common Elective Course and Discipline Specific Elective Courses* designed for individual Chemical science whereas, a research scholar will select elective courses as suggested by the concerned DRC. Evaluation of the research plan proposal and presentation, and review of literature will be done by the concerned DRC. The detailed course layout is given below.

Course Structure:

(A) Common Courses (05 credits)

Course Code	Title	Nature	Credits
CHM T 700	Research Methodology	Compulsory	**04**
CHM P 700	Lab. work based on CHM T 700	Compulsory	**01**

(B) Research Them- Common Elective Course (opt any one) (04 credits)

S. No.	Course Code	Course Structure	Title	Credits
1	CHM T 701	Elective	Principles of Physical Chemistry	**04**
2	CHM T 702	Elective	Modern Physical Methods in Chemistry Research	**04**
3	CHM T 703	Elective	Nanomaterials: Synthesis and Characterization	**04**
4	CHM T 704	Elective	Newer Methods in Organic Synthesis	**04**
5	CHM T 705	Elective	Supramolecular Chemistry	**04**

(C) Research Them – Discipline Specific Elective Courses (06 Credits)

Discipline Specific Elective Course* (Opt any one)			
Course Code	**Course Structure**	**Title of Paper**	**Credit**
CHM T 801	Elective	Advanced Analytical Chemistry	04
CHM P 801	Lab	Advanced Analytical Chemistry Lab	02
CHM T 802	Elective	Advanced Organometallic Chemistry	04
CHM P 802	Lab	Advanced Organometallic Chemistry Lab	02
CHM T 803	Elective	Advanced Materials Chemistry	04
CHM P 803	Lab	Advanced Materials Chemistry Lab	02
CHM T 804	Elective	Nanoscience & it's Applications	04
CHM P 804	Lab	Nanoscience & it's Applications Lab	02
CHM T 805	Elective	Polymers Chemistry	04
CHM P 805	Lab	Polymers Chemistry Lab	02
CHM T 806	Elective	Bioorganic and Drug Chemistry	04
CHM P 806	Lab	Bioorganic and Drug Chemistry Lab	02
CHM T 807	Elective	Advanced Heterocyclic Chemistry	04
CHM P 807	Lab	Advanced Heterocyclic Chemistry Lab	02
CHM T 808	Elective	Chemistry of Natural Products	04
CHM P 808	Lab	Chemistry of Natural Products Lab	02
CHM T 809	Elective	Advanced Synthetic Organic Chemistry	04
CHM P 809	Lab	Advanced Synthetic Organic Chemistry Lab	02
CHM T 810	Elective	Principles of X-ray Diffraction and Electron Microscope	04
CHM P 810	Lab	Principles of X-ray Diffraction and Electron Microscope Lab	02

*** Notes:**

- **Research scholars those who studied above mentioned courses in their PG Programme they must opt different course.**
- **All the elective papers will be offered as suggested by the concern DRC.**

CHM T 700: Research Methodologies

Credits: 04
Theory: 60 Hours

1. An overview of research methodology: Research concept, steps involved, identification, selection and formulation of research problem, justification, hypothesis; literature collection- textual and digital resources (internet)
2. Research design, data collection and interpretation: Research design; sampling techniques, collection and documentation, presentation, analysis and interpretation of data
3. Scientific writing: Forms of scientific writing- Article, notes, reports, review article, monographs, dissertations, popular science articles, bibliographies,
4. Formulation of scientific communication - Outline preparation, drafting title, sub titles, tables, illustrations; Formatting tables- title, body footnotes; figures & graphs- structure, title and legends, Impact factor, citation indices, plagiarism
5. Computer application: MS office, excel, power point, graphics (Origin), statistical software (SPSS), CHEMDRAW, Full Prof *etc*.
6. Statistics: Standard deviation/error; Correlation coefficient, types of correlation, regression equation, Test of significance, chi-square test, analysis of variance

Suggested Readings:

- Research Methodology - Methods & Techniques, CR Kothri CR (1990), Vishva Prakashan, New Delhi.
- Research Methodology & Statistical Techniques, S Gupta (1999) Deep & Deep Publications, New Delhi.
- Research methodology for biological sciences, N Gurumani (2007), MJP Publishers, Chennai.
- Introduction to Biostatistics, L Forthofer (1995), Academic Press, New York.
- Biostatistical Analysis, JH Zar (2006), Prentice-Hall.
- Research Design: Qualitative, Quantitative & Mixed Method Approaches. John W. Creswell (2009), Sage Publication, USA.
- Experimental Design & Data Analysis for Biologists. PQ Gerry & JK Michael (2002), Cambridge University Press.
- Choosing and Using Statistics: A Biologists Guide, D Calvin (2003), Blackwell Publisher.

CHM T 701: Principles of Physical Chemistry

Credits: 04
Theory: 60 Hours

Unit – 1: Quantum Chemistry-I

Historic Background, Schrödinger wave Equation, operators, and solution of the Schrödinger equations for some exactly soluble systems: particle-in-a-box; particle-in-a-ring and -sphere; harmonic oscillator; tunneling one dimensional potential barrier and well, rigid rotor, and hydrogen and H-like atoms.

(12 Hours)

Unit– 2: Quantum Chemistry-II

Angular momentum, approximation methods of quantum chemistry, and atomic structure and spectroscopy.

(12 Hours)

Unit – 3: Chemical Bonding and *Ab-initio* Methods

***Chemical Bonding*:** Elementary concepts of MO and VB theories; Born-Oppenheimer approximation, MO treatment for H_2^+ ion, MO treatment of homo- and hetero- nuclear diatomic molecules; comparison of MO and VB theories. Hückel MO theory for conjugated π-systems. Polyatomic molecules, hybridisation and valence MOs of simple molecule like H_2O, NH_3, CH_4, C_2H_6 *etc*.

***Ab-initio* methods:** Introductory treatment of semi-empirical and *ab-initio* calculations on molecular systems; the Hartree-Fock Self-Consistent Field Method; the generation of optimized orbitals, Koopman's theorem (The Physical Significance of Orbital Energies), electron correlation energy; density matrix analysis of the Hartree-Fock approximation, natural orbitals, matrix solution of the Hartree-Fock equations (Roothaan's equations); Hellman-Feynman theorem.

(12 Hours)

Unit – 4: Statistical Thermodynamics

Concept of distribution, thermodynamic probability and most probable distribution. Corresponding distribution laws (using Lagrange's method of undetermined multipliers). Partition function ; Applications of partition functions.

Heat capacity behavior of solid – chemical equilibria and equilibrium constant in term of partition function. Fermi-Dirac statistics, distribution law and application to metal, Bose-Einstein statistics, distribution law and application to helium.

(12 Hours)

Unit – 5: Chemical Kinetics and Catalysis

Rate law, method of determining rate laws, General feature of fast reactions, study of fast reaction by flow method, relaxation method, flash photolysis and the nuclear magnetic resonance method.

Reactions in Gas Phase: Theories of Reaction Rates- Arrhenius theory, collision theory and transition state theory; uni-molecular reactions.

Elementary Reactions in Solution**:** Comparison between gas-phase and solution-phase reactions, factor determining reaction rates in solution; ionic reaction [influence of solvent, influence of ionic strength (salt effect)]

Heterogeneous and Homogeneous Catalysis**:** Kinetics of uni-molecular reactions- inhibition and activation energy. Bimolecular surface reactions, enzymatic reactions, acid – base catalysis

(12 Hours)

Reference Books:

- Ira. N. Levine: Quantum Chemistry, Eds: 5th, PHI, 2000.
- A. K. Chandra: *Introductory Quantum Chemistry*, Eds: 4th, Tata McGraw Hill, New Delhi, 1994.
- P. Atkins and R. Friedman: *Molecular Quantum Mechanics*, Eds: 5th, Oxford University Press, 2011.
- T. Engle and P. Reid: *Quantum Chemistry and Spectroscopy*, Pearson, New Delhi, 2011.
- B. R. Puri, L. R. Sharma and M. S. Pathania, *Principle of Physical Chemistry*, Eds. 44th, Vishal Publishing Co., Jalandhar, 2010.
- P. Atkins and J. D. Paula, *Physical Chemistry*, Eds. 7th, Oxford University Press, New Delhi, 2002.
- R. S. Berry, S. A. Rice and J. Ross: P*hysical Chemistry*, Eds: 2nd, Oxford University Press, New Delhi, 2007.
- K. J. Laidler, *Chemical Kinetics*, Eds: 3rd, Pearson, 2011.
- J Rajaram and J. C. Kuriacose: *Kinetics and Mechanisms of Chemical Transformations Applications of Femto-chemistry*, MacMillan, New Delhi, 2011.

CHM T 702: Modern Physical Methods in Chemistry Research

Credits: 04
Theory: 60 Hours

Unit – 1: General Principles

Electromagnetic radiation, interaction of electromagnetic radiation with matter, absorption, emission, transmission, reflection, refraction, dispersion, polarization, and scattering. Uncertainty relation and natural line width and natural line broadening, transition probability, result of the time dependent perturbation theory, transition moment selection rules, intensity of spectral line. Born-Oppenheimer approximation, rotational, vibrational, and electronic energy levels. Fourier Transform Spectroscopy.

(12 Hours)

Unit – 2: Rotational and Vibrational Spectroscopy

Review of Microwave, Infrared Spectroscopy, FTIR, and Raman Spectroscopy

(12 Hours)

Unit – 3: Electronic Spectroscopy and Magnetic Resonance Spectroscopy

Electronic Spectroscopy: Atomic Spectroscopy Molecular Spectroscopy and Photoelectron Spectroscopy

Magnetic Resonance Spectroscopy: Nuclear Magnetic Resonance Spectroscopy; Electron Spin Resonance Spectroscopy; Nuclear Quadrupole Resonance Spectroscopy

(12 Hours)

Unit – 4: X-ray Diffraction and Mossbauer Spectroscopy

X-ray Diffraction: Bragg condition, miller indices, Laue method, Bragg Method, Debye-Scherrer method of X-ray structural analysis of crystals, index reflections, identification of unit cells from systematic absence in diffraction pattern. Structure of simple lattice and X-ray intensity, structure factor and its relation to intensity and electron density phase problem. Description of the procedure of an X-ray structure analysis.

***Mössbauer Spectroscopy*:** Basic principles, spectral parameters and spectrum display. Application of technique to the studies

(14 Hours)

Unit – 5: Microscopy

Electron microscopy (SEM, TEM with EDX analysis). A brief historical overview of atomic force microscopy (AFM).

(10 Hours)

Reference Books:

- C. N. Banwell and E. M. McCash: *Fundamentals of Molecular Spectroscopy*, Ed. 4th, Tata McGraw-Hill, 1994.
- B. D. Cullity: *Elements of X-ray Diffraction*, Eds: 2nd, Addison-Wesley, USA, 1959.
- D. B. Williams and C. B. Carter: *Transmission Electron Microscopy: A Textbook for Materials Science*, Plenum Press, New York, 1996.
- S. Hüfner: *Photoelectron Spectroscopy: Principles and Applications*, Springer-Verlog, Germany, 1995.

CHM T 703: Nanomaterials: Synthesis and Characterization

Credits: 04
Theory: 60 Hours

Unit – 1: Nanoscience and Nanotechnology

***Introduction*:** Underlying physical principles of nanotechnology: *Nanostructured Materials: Size is Everything*. Fundamental physicochemical principles, size and dimensionality effects; quantum confinement; properties dependent on density of states; single electron charging, central importance of nanoscale morphology.

***Type of Nanostructures*:** Definition of a nano system; one dimensional (1D), two dimensional (2D), three dimensional (3D) nanostructured materials; quantum dots; quantum wire, and core/shell structures.

(12 Hours)

Unit – 2: Some Important Nanomaterials

Variety of inorganic (traditional to advanced) materials, Importance of Structural/refractory, Electronic and Bio-materials, Oxide superconductors and novel materials. Description of crystals, Bonding, Inorganic structures, Silicates and Alluminosilicates, Polytypism, Nanocrystalline/amorphous solids.

(12 Hours)

Unit – 3: Characterization Techniques

X-ray diffraction, electron microscopy (SEM, TEM, AFM), thermal techniques (TG, DTA, DSC), spectroscopic techniques (Mössbauer, IR, UV-VIS), and physical property measurement techniques (magnetic moments-VSM/SQUID, electrical resistivity – two / four probe methods and thermal conductivity, optical band gap, XPES, XAS.

(12 Hours)

Unit – 4: Chemical Routes Preparation Techniques

***Chemical Routes for Synthesis of Nanomaterials*:** Chemical precipitation and co-precipitation; sol-gel synthesis; microemulsions or reverse micelles; solvothermal synthesis; thermolysis routes, microwave heating synthesis biomimetic and electrochemical approaches; sonochemical synthesis; photochemical synthesis; synthesis in supercritical fluids.

(12 Hours)

Unit – 5: Applications of Nanomateirals

Journal paper presentation from any recent work of metal, metal oxide and metal nitride based nanomaterials.

(12 Hours)

Reference Books:

- D. Segal: *Chemical Synthesis of Advanced Ceramic Materials*, Cambridge Univ. Press, Meew York 1989.
- L. L. Hench and J. K. West (eds): *Chemical Processing of Advanced Materials*, John Wiley New York 1992.
- P. Hagnmuller (ed): *Preparative Methods in Solid State Chemistry*, Acdemic Press, New York, 1972.
- C. J. Brinker & G. W. Scherer: *Sol-Gel Science*, Academic Press, 1980.
- *Non-Oxide Technical & Engg. Ceramics*, Ed. Stuart Hampshire, Elsevier Applied Science Pub. Ltd. 1986.

CHM T 704: Newer Methods in Organic Synthesis

Credits: 04
Theory: 60 Hours

Unit – 1: Metal Mediated C-C and C-X Coupling Reactions

Suzuki, Heck, Negishi, Stille, Sonogishira cross coupling, Buchwald-Hartwig and Negishi-Kumada coupling reactions. **C=C Formation Reactions:** Shapiro, Bamford-Stevens, McMurrey reactions, Julia Lythgoe olefination and Peterson's stereoselective olefination. Olefin metathesis by I^{st} and II^{nd} generation catalysts: Reaction mechanism and application in the synthesis of heterocycles.

(12 Hours)

Unit – 2: Organometalic Compounds and Application in Organic Synthesis

Organomagnesium, Organolithium, Organozinc and Organocopper reagents preparation and applications in organic synthesis. Chemistry of Phosphorous, Sulfur, Silicon, Boron and Tin compounds and application in organic reactions.

(12 Hours)

Unit – 3: Disconnection Approach, Umpolung Chemistry and Protection-Deprotection of Functional Groups

Basic principles and terminology of Target molecule, FGI, Disconnection, Synthon, Reagent and Retro-synthetic approach. **One group C-C and C-X disconnection**: (disconnection of alcohols, alkenes, and carbonyl compounds). **Two group C-C & C-X disconnections**: 1,3 and 1,5 difunctionalised compounds, α, β, unsaturated carbonyl compounds, control in carbonyl condensation, synthesis of 3,4,5 and 6 membered rings in organic synthesis. Diels-Alder reaction, connection in retro synthesis. Umpolung chemistry in organic synthesis. Protection and deprotection for functional groups as hydroxyl, amino, carboxylic and carbonyl.

(12 Hours)

Unit – 4: Selective Stereoselective Organic Reactions with Alkenes and A Few Methods for Asymmetric Reactions

Sharpless Asymmetric Epoxidation, Asymmetric Aziridination, Dihydroxylation, Amino-hydroxylation Reactions, A few popular privileged chiral ligands: applications in organic reactions, Organocatalysis: chiral secondary amine, phosphine and NHC catalyzed asymmetric reactions.

Unit – 5: Journal paper presentation from any recent work in organic chemistry journals.

(12 Hours)

Reference Books:

- B. F.G. Johnson, *Transition metal cluster*, Wiley, 1980.
- R. H. Crabtree, *The Organometallic Chemistry of the Transition Metals*, Wiley-Interscience, 2005.
- G. Wikinson, F. G .A. Stone, E. Abel, *Comprehensive Organometallic Chemistry*, Peramon, 1980.
- I. Fleming, *Frontier Orbitals and Organic Chemical Reactions*, Wiley, 1976.

- S. Warren, Organic Synthesis: T*he Disconnection Approach*, John Wiley & Sons (Asia) Pte. Ltd., 2007
- W. Carruthers and I. Coldham: *Modern Methods of Organic Synthesis*, Fourth Ed. Cambridge University Press.
- For Unit 05, the students are advised to select journal from ACS or Willey Publishers for the presentation.

CHM T 705: Molecular recognition and Supramolecular Chemistry

Credits: Theory-04
Theory: 60 Hours

Unit – 1: Principal of molecular recognition

Concept of molecular recognition and Supramolecular Chemistry. Host-Guest Chemistry, and its classification. Receptor, Coordination and the lock and key analogy. Thermodynamic and Kinetic Selectivity. Nature of supramolecular interactions.

(10 Hours)

Unit – 2: Supramolecular Chemistry of Life

Alkali metal ions in biochemistry. Porphyrins and Tetrapyrrole macrocycles. Plant Photosynthesis. Uptake and transport of oxygen in Haemoglobin. Coenzyme B_{12}.Neurotransmitter and Hormones. DNA. Biochemical self assembly.

(10 Hours)

Unit – 3: Cation & Anion Binding Host

Crown ether, Lariat ether and podands, Cryptands, Calix[n]arenes; Spherands; Selectivity of cation complexation; Macrocyclic, Macrobicyclic and Template effect.

Concept of Anion binding host design. Guanidium-based receptors; Organometalic receptors; Neutral receptors, Hydride sponge; Anticrown; Biological anion receptors.

(20 Hours)

Unit – 4: Binding of Neutral molecules

Binding by cavitands, cyclodextrines, Molecular cleft and tweezers, cyclophanes, cryptophanes Host.

(10 Hours)

Unit – 5: Supramolecular reactivity and Catalysis

Catalysis by cation, anion and neutral receptors; Supramolecular metallocatalysis; Cocatalysis; Biomolecular and abiotic cataysis.

(10 Hours)

Reference Books:

1. J. W. Steed and J. L. Atwood: *Supramolecular Chemistry*, John Wiley and Sons, Ltd.
2. Jean –Marie Lehn: *Supramolecular Chemistry-Concepts and Perspectives*, VCH.
3. Hans-Jorg Schnider and Anatoly K. Yatsimirsky: *Principles and Methods in Supramolecular Chemistry*, John Wiley and Sons, Ltd.
4. Antonio Bianchi, Kristin Bowman James and Enrique Garcia-Espana: *Supramolecular Chemistry of anions*, Wiley-VCH.

Discipline Specific Elective Course* (opt any one)

CHM T 801: Advanced Analytical Chemistry

Credits: Theory-04
Theory: 60 Hours

Unit – 1: Advanced Molecular Spectroscopy & Data Interpretation

Nature of electromagnetic radiation, electromagnetic spectrum, atomic, molecular and vibrational energy levels, basic instrumentation- source of radiation, monochromator, sample cells, absorber, detector, UV-Vis detector, photomultiplier, IR detector, display and recorder, single and double beam spectrophotometer, Beer Lambert law, deviation from beers law, ultraviolet and visible spectroscopy, Fluorescence and phosphorescence spectrophotometer, Fourier transform infrared spectrometer and Raman spectrometer, instrumentation, techniques and application.

Errors and Statistics: significant figures, rounding off, accuracy and precision, determinate and indeterminate errors, standard deviation, propagation of errors, confidence limit, test of significance, rejection of a result.

(12 Hours)

Unit – 2: Thermal Analysis & Atomic Spectroscopy

Types of thermal method, Thermogam, thermogravimetric analysis(TGA), differential thermal analysis(DTA), differential scanning calorimetry (DSC), schematic diagram for TGA and DTA instruments and their working principle, factors affecting thermogram like geometry of sample holder, furnace atmosphere, heating rate, particle size, packing of sample, weight of sample, analysis of metals or oxide in mixture, application of TGA and DTA.
Flame emission spectrometry, atomic absorption spectroscopy- principle, instrumentation, Source in AAS – Hollow cathode lamp, electrode less discharge lamp, burners, nature and property of flame, interference in AAS, difference between AAS and FES, ICP.

(12 Hours)

Unit – 3: Purification Technique

Chromatography

Principles of chromatographic separation, classification of Chromatographic Techniques: adsorption, partition, ion exchange and size exclusion chromatography, theory of chromatographic separation, distribution coefficient, retention time, sorption, theory of column efficiency and resolution, separation factor, retention factor. – working principle and application of Column chromatography, ion exchange chromatography, paper chromatography, Thin layer chromatography (TLC) & HPTLC: techniques and application. - Gas Chromatography and high performance liquid chromatography: Van Deemter equation, retention time or volume, capacity ratio, partition coefficient, theoretical plate and number, separation efficiency and resolution, instrumentation and application.

Solvent extraction

Theory, efficiency, percentage extraction, separation factor, complexing agent in solvent extraction, selection of solvent.

Ion- exchange
Principle, quality of resins, ion exchange equilibrium, ion exchange capacity process, deionization of water.

(14 Hours)

Unit – 4: Electrochemical analyses

Introduction to electrochemical methods, electrochemical cells, diffusion controlled limiting current, voltage scanning polarography, shape and interpretation of polarographic wave, limiting current, current – voltage relationship during electrolysis. Electrogravimetry, voltammetry, polarography, reference electrode, working electrode, auxiliary electrode, dropping mercury electrode, Principles and applications of Voltammetry, cyclic voltammetry, polarography, anodic stripping voltammetry, amperometry, coulometry, electrogavimetry.

(12 Hours)

Unit – 5: Gravimetric Analysis & Quantitative Estimation

Advantage of gravimetric analysis, requirement, preparation of solution, precipitating reagent, condition for analytical precipitation, saturation and super-saturation, von Weimarn equation, co-precipitation, digestion, Ostwald ripening, aggregation and agglomeration, colloidal solution, adsorption, primary and secondary layer adsorption, peptization, impurity, inclusion and occlusion, surface adsorption, post precipitation, filtration, washing and weighing precipitate mathematical calculation on gravimetry.

Basic principle of acid base indicator, Redox titration- titration of Mohr salt against $KMnO_4$, complexometric titration- EDTA titration, Eriochrome black T indicator, complexometric titration curve, direct and back titration, masking and demasking of cations, precaution in volumetric titration, titration & Justification of Fe^{3+} and Mn^{2+} salt both in complexometry and Spectrophotometry analysis.

(10 Hours)

Reference Books:

- D. C. Harris, Quantitative Chemical Analysis, 4th Ed., W. H. Freeman, 1995
- G. D.Christian & J. E. O'Reily, Instrumental Analysis, 2nd Ed., Allyn & Balon, 1986.
- I. Vogel: *A Test book of Quantitative Inorganic Analysis* (Rev. by G.H. Jeffery and others) 5th Ed. The English Language Book Society of Longman .
- Hobert H. Willard et al: *Instrumental Methods of Analysis*, 7th Ed. Wardsworth Publishing Company, Belmont, California, USA, 1988.
- Gary D. Christian: *Analytical Chemistry*, 6th Ed. John Wiley & Sons, New York, 2004.
- C. Daniel Harris: *Exploring Chemical Analysis*, Ed. New York, W.H. Freeman, 2001.
- S. M. Khopkar: *Basic Concepts of Analytical Chemistry*, New Age, International Publisher, 2009.
- D. A. Skoog, F. J. Holler and T. A Nieman: *Principles of Instrumental Analysis*, Thomson Asia Pvt. Ltd. Singapore.

- O. Mikes & R. A. Chalmes: *Laboratory Hand Book of Chromatographic & Allied Methods*, Elles Harwood Ltd. London.
- R. V. Ditts: *Analytical Chemistry* – Methods of separation.

CHM P 801: Advanced Analytical Chemistry Lab

Credit: 02
(Lab: 60 Hours)

Group-A: Analysis of Complex Materials

Quantitative analysis of complex materials, such as, ores and minerals, metals and alloys, industrial materials by conventional and or instrumental methods as applicable.

Model Samples

Ores, Minerals , Concentrates*:* Dolomite ($CaCO_3$, Mg CO_3, Fe_2O_3, SiO_2); Pyrolusite (MnO_2, MnO, Fe_2O_3); Chalcopyrite (CuS, FeS); Bauxite (Al_2O_3, Fe_2O_3, TiO_2, SiO_2); Chromite (Cr_2O_3, Fe_2O_3, MnO, SiO_2); Basic slag (Al_2O_3, Fe_2O_3, P_2O_5, SiO_2).

Metals and Alloys: Brass (Cu, Zn); Soldier / Type metal (Pb, Sb, Sn); Bronze(Cu, Zn, Sn), Aluminium bronze(Cu, Al, Fe, Mn), Steel (Cr, Mn, Ni, P).

Mixture: Chromium (III) and Mn(II) in a mixture, Iron (III) and Cu(II) in a mixture, Iron(III) and Al(III) in a mixture

At least one ore/ mineral/concentrate and one alloy should be analyzed during the laboratory session.

Group-B: FT-IR and UV assignment of synthesized metal complexes

Reference Books:

- I. Vogel: *A Test book of Quantitative Inorganic Analysis* (Rev. by G.H. Jeffery and others) 5th Ed. The English Language Book Society of Longman .
- Hobert H. Willard et al: *Instrumental Methods of Analysis*, 7th Ed. Wardsworth Publishing Company, Belmont, California, USA, 1988.
- Gary D. Christian: *Analytical Chemistry*, 6th Ed. John Wiley & Sons, New York, 2004.

CHM T 802: Advanced Organometallic Chemistry

Credits: Theory-04
Theory: 60 Hours

Unit – 1: Organometallics

Compounds with metal carbon σ and multiple bond: Haptacity complexes of Metal-alkyl, -allyl, aryl, -carbene (Fischer and Schrock type), -carbonyl, -carbines and cyclopentadienyl complexes Synthesis, bonding, stability, reactivity and decomposition pathway, Reactions in organometallic compounds. Stucture and bonding in η^2-ethylenic and η^3-allylic compounds with typical examples, structure and bonding of $K[Pt(C_2H_4)Cl_3]$, $[(Ph_3P)_2Pt(Ph\text{-}C{\equiv}C\text{-}Ph)]$. Fluxional organometallic compounds: Fluxionality and dynamic equilibria in compounds such as η^2 olefins, η^3 allyl and dienyl complexes, techniques of study.

Reactions of organometallic complexes: substitution, oxidative addition, reductive elimination, insertion and elimination, electrophilic and nucleophilic reactions of coordinated ligands.

(12 Hours)

Unit – 2: **Catalysis**

Catalysis by organometallic compounds: Hydrogenation of olefins, Wilkinson's catalyst, Tolman catalytic loop; synthesis gas, water-gas shift reaction; Hydroformylation (oxo process), Monsanto acetic acid process, Wacker process; synthetic gasoline: Fischer-Tropsch process and Mobile process, polymerization, oligomerization and metathesis reactions of alkens and alkynes, Zieglar- Natta catalysis, photo dehydrogenation catalyst (platinum POP).

(12 Hours)

Unit – 3: Inorganic Heterocyclic & Homocyclic Rings

P-N rings: Cyclophosphazenes, Synthesis, structure and Reactivity, Bonding models
P-N-X rings: carbophosphazenes, thiophosphazenes, metallaphosphazenes
Si-O rings: Cyclosiloxanes
Sn-O rings: Stannoxanes
Al-containing Rings: Al-N rings and cages, Al-C rings and cages, Alumoxanes

Inorganic homocyclic rings and cages containing silicon, germanium , boron, aluminum and gallium

Unit – 4: Recent Developments in Organometallics Chemistry Research

Construction, structure and property of compounds with specific topology in Organometallic Chemistry: Capsules, boxes, containers, prisms or clusters, tubes, catenanes, rotaxanes, incorporation of metal atoms through metal-ligand coordination interactions, Various organic ligands containing carboxy, imidazole or pyridine groups, which can coordinate with metal atoms, have been used to generate the desired compounds (V, Cr, Mn, Fe, Co, Ni, Cu). Particularly, flexible ligands with central aromatic core and imidazol-1-ylmethyl pendant arms, e.g. 1,3,5-tris(imidazol-1-ylmethyl)-2,4,6-trimethylbenzene and its analogues,

Interesting properties: Molecular recognition, ion inclusion and exchange of these compounds, especially of the cage-like compounds, are described.

(12 Hours)

Unit – 5: Inorganic Cages and Clusters

Polymorphism of C, P and S. Structure and bonding in higher boranes and borohydrieds-Lipscomb's topological models, Wade`s rules, carboranes and metallocenecarboranes.

Metal-metal bonding (M.O. Approach), metal-metal single and multiple bonded compounds. Low nuclearity (M_3, M_4) and high nuclearity (M_5-M_{10}) carbonyl clusters: skeletal electron counting, Wade-Mingos-Louher rule, Application of isolobal and isoelectronic relationships, Nb and Ta clusters, Mo and W clusters. Cluster compounds in catalysis.

(12 Hours)

Reference Books:

- J. E. Huheey, E. A. Keiter, R. L. Keiter, and O. K. Medhi: *Inorganic Chemistry Principle of Structure and Reactivity*, Eds: 4th Pearson, New Delhi, 2006.
- F. A Cotton, G. Wilkinson, C. A. Murillo, and M. Bochmann: *Advanced Inorganic Chemistry*, Eds: 6th, Wiley-India, New Delhi, 2010.
- D. F. Shriver and P. W. Atkins: *Inorganic Chemistry*, Oxford University Press.
- Douglas, McDaniel and Alexader: *Concepts and Models in Inorganic Chemistry*, John Wiley.
- Robert Crabtree: *The Organometallic Chemistry of the Transition Metals*, 3rd Edition, Wiley.
- Collman, Hegedus, Norton and Finke: *The Principles and Applications of Transition Metal Chemistry*, 2nd Eds, University Science Books.
- Christoph Elschenbroich: *Organometallics*, 3rd Edition,
- Wei-Yin Sun, *New Developments in Organometallics Chemistry***,** Wiley

CHM P 802: Advanced Organometallic Chemistry Lab

Credit: 02
(Lab: 60 Hours)

A. Preparation of selected inorganic compound and their studies by I.R., electronic spectra, Mössbauer and magnetic susceptibility measurements. Handling of air and moisture sensitive compounds

1. Mn_{12} Acetate Single Molecule Magnets
2. $K_2[Fe(C_2O_4)_3]$ .3 H_2O
3. $[Fe_3(\mu_3\text{-}O)(\mu\text{-}O_2CR)_6L_3]$ (L = H_2O, R= alkyl/aryl/)
4. $[Fe_3O(PhCO_2)_6(MeOH)_3](NO_3)(MeOH)_2$
5. $[Fe_8O_3(O_2CCMe_3)_6(N_3)_3(tea)(teaH)_3]\cdot 0.5(EtOH)$
6. $Cu_2(C_6H_5COO)_4(C_6H_5COOH)_2$
7. Tris(ethylenediamine)nickel(II) thiosulphate

B. Determination of crystal Structure by ORTAP file.

References Books:

- Liz, T. *Acta Crystallogr.* ***1980***, *B36*, 2042
- Sessoli, R.; Tsai, H.-L.; Schake, A. R.; Wang, S.; Vincent, J. B.; Folting, K.; Gatteschi, D.; Christou, G.; Hendrickson, D. N. J. Am. Chem. Soc. 1993, 115, 1804.
- J-X. Daia, F-H. Wua, A. Rothenbergerb, Q-F. Zhang, *Z. Naturforsch.*, 2007, 62b, 1117 – 1122.
- M. K. Zart, D. Powell, A. S. Borovik, *Inorganica Chimica Acta*. 2007, 360(7), 2397–2402.
- V. Psycharis, C. P. Raptopoulou, A. K. Boudalis, Y. Sanakis, M. Fardis, G. Diamantopoulos, G. Papavassiliou, *Eur. J. Inorg. Chem.*, 2006, 3710–3723.
- M. Narshim, A. Saritha, B. Raju, K. A. Hussain, IJIRSET, 4(8), 2015, 7548-7555.
- Olga Botezat, Jan van Leusen, Victor Ch. Kravtsov, Arkady Ellern, Paul Kögerler and Svetlana G. Baca, Dalton Trans., 2015, 44, 20753.
- S. Pathak, N. Biswas, B. Jana, T. K. Ghorai, Advanced Materials proceeding, 2017

CHM T 803: Advanced Materials Chemistry

Credits: Theory-04
Theory: 60 Hours

Unit – 1: Chemical Crystallography

***Introduction*:** Space lattice, crystal point groups, space group (working knowledge), stereographic projections, packing in solids, crystal structures of representative systems, silicates and zeolites, cements, glasses, quasicrystals, nanostructures.

***Bonding in Solids and Crystal Energetics*:** Crystal classifications, Madelung constant and Lattice energy.

(12 Hours)

Unit – 2: Characterization Techniques for Solids

X-ray diffraction, electron microscopy (SEM, TEM, AFM), thermal techniques (TG, DTA, DSC), spectroscopic techniques (Mössbauer, IR, UV-VIS), and physical property measurement techniques (magnetic moments-VSM/SQUID, electrical resistivity – two / four probe methods and thermal conductivity, optical band gap, XPES, XAS.

(12 Hours)

Unit – 3: Electronic and Magnetic Properties Solids

Electronic Properties and Band Theory of Solids: Free electron theory of metals, Band theory of solids, Bloch theorem, Kroning-Penne model, refinement of simple band theory- *k*-space and Brillouin Zones, band structure of metals, insulators and semiconductors, intrinsic and extrinsic semiconductors, doped semiconductors, *p-n* junctions.

***Magnetic Properties Solids*:** Behaviour of substances in a magnetic field, effect of temperature: Curie and Curie-Weiss law, origin of magnetic moment, ferromagnetic, antiferromagnetic and ferromagnetic ordering, super exchange, magnetic domains, hysteresis. Introduction of superconductors, Meissner effects, basic concepts of BCH theory.

Unit – 4: Defects and Phase Transitions

***Defects, Nonstoichiometry and Diffusion*:** Point defects, dislocations, extended defects, clusters and aggregates, color centers, nonstoichiometry of compounds, diffusion mechanisms, Fick's law, Kirkenall effect.

***Phase Transitions*:** Critical phenomena, variety of phase transitions (ordered-disorder, Martensite-austenite, spinoidal decompositions *etc*), liquid crystals, structure-property relations (magnetic, electrical, superconductivity, optical and thermal).

Unit – 5: Preparative Techniques

***Reactivity of Solids*:** Decomposition and reactivity, solid state reactions, sintering process, reaction kinetics, organic solid reactions.

***Conventional Techniques*:** Powder mixing, fusion, precipitation from solution, modern need for improved synthetic routes, crystal growth and thin film techniques.

Chemical Routes: Wet-chemical (Oxidation-reduction for metal nanoparticles) methods, self assembly methods, reverse micelles route, biomimetic, sonochemical, and electrochemical approaches.

***Sol-Gel Synthesis*:** Colloids, cation hydrolysis and sol formation, gel precipitation, sol-gel process for colloids, synthesis andphysical properties of metal alkoxides, development of sol-gel process from alkoxides, derived coatings, fibers and monodispersed submicron/ nanostructured oxide powders, ormosils, sialons.

***Hydrothermal/Solvothermal Approach*:** Forced hydrolysis at elevated temperatures and pressures, hydrothermal reactions using salt solutions, metal reactants and reactions involving phase transformation.

***Precursor Technique*:** Citrate-gel process, metallo-organic precursors, metal alkoxides.

***Gas Phase Reactions*:** Gas-phase nucleation, flame hydrolyzed powders, direct - nitridation and carbothermic reduction, non-plasma gas phase reactions, plasma reactions, electron beam evaporation.

(12 Hours)

Reference Books:

- A. R. West: *Solid State Chemistry and Its Applications*, John Wiley & Sons, 1989.
- L. Smart and E. Moore, *Solid State Chemistry*, Chapman and Hall, 1992.
- A. K. Cheetham and P. Day: *Solid State Chemistry Compounds*, Clarendon Press, Oxford 1992.
- C. N. R. Rao and J. Gopalkrishanan: *New Directions in Solid State Chemistry*, Cambridge Univ. Press 1997.
- R. E. Newnham, *Structure Property Relations*, Springer-Verlag, 1987

CHM P 803: Advanced Materials Chemistry Lab

Credits: 02
(60 Hours)

1. Synthesis of Mixed alloy oxide (Fe_2O_3/TiO_2, Fe_2O_3/ZnO, Fe_2O_3/ZrO_2)
2. Characterization of synthesizes materials: UV, FTIR, XRD, Electron Microscopy (available of Department)
3. Application Study: Ellectric, Magnetic, Catalytic etc.
4. Presentation / Seminar
5. Literature Review report

CHM T 804: Nanoscience & it's Applications

Credits: Theory-04
Theory: 60 Hours

Unit – 1: Nanoscience and Nanotechnology

***Introduction*:** Underlying physical principles of nanotechnology: *Nanostructured Materials: Size is Everything*. Fundamental physicochemical principles, size and dimensionality effects; quantum confinement; properties dependent on density of states; single electron charging, central importance of nanoscale morphology. Societal aspects of nanotechnology: health, environment, hype and reality.

***Type of Nanostructures*:** Definition of a nano system; one dimensional (1D), two dimensional (2D), three dimensional (3D) nanostructured materials; quantum dots; quantum wire, and core/shell structures.

(12 Hours)

Unit -2: The Basic Tools of Nanotechnology

Electron microscopy (SEM, TEM with EDX analysis) and X-ray diffraction, A brief historical overview of atomic force microscopy (AFM); an introduction and basic principles & applications of XPS, FTIR spectrophotometers; UV-VIS principle and application for band gap measurement.

(12 Hours)

Unit – 3: Synthesis of Nanomateirals

Top down and bottom up approaches to synthesis of nanomaterils:

***Chemical Routes for Synthesis of Nanomaterials*:** Chemical precipitation and co-precipitation; sol-gel synthesis; microemulsions or reverse micelles; solvothermal synthesis; thermolysis routes, microwave heating synthesis biomimetic and electrochemical approaches; sonochemical synthesis; photochemical synthesis; synthesis in supercritical fluids.

***Physical Routes for Preparation of Nanomaterial*:** Inert gas condensation, arc discharge, RF plasma, plasma arc technique, ion sputtering, laser ablation, laser pyrolysis, spray pyrolysis, ball milling, molecular beam epitaxy, chemical vapour deposition method, Langmuir-Blodgett (LB) films, spin coating and electro deposition.

(12 Hours)

Unit – 4: Nanomateirals and Properties

Synthesis and size dependent properties (mechanical, physical and chemical properties) of carbon nanotubes (CNT); metals (Au, Ag); metal oxides (TiO_2, CeO_2, ZnO); semiconductors (Si, Ge, CdS, ZnSe); dilute magnetic semiconductor.

(12 Hours)

Unit -5: Applications of Nanomateirals

Basic ideas of nanodevices (molecular electronics and nanoelectronics, and quantum electronic devices); CNT based transistor and field emission display; biological applications;

biochemical sensor; membrane based water purification, energy storage devices, catalysis and various related fields.

(12 Hours)

Reference Books:

- T. Pradeep, *Nano: The Essentials*, Tata McGraw-Hill, New Delhi, 2007.
- G. Cao, *Nanostructures and Nanomaterials – Synthesis, Properties and Applications*, Imperial College Press, London, 2004,
- C. N. R. Rao, A. Muller and A. K. Cheetham, *The Chemistry of Nanomaterials*
- G. L. Hornyak, J. J. Moore, H. F. Tibbals, and J. Dutta: *Fundamentals of Nanotechnology*, CRC Press, 2009

CHM P 804: Nanoscience & it's Applications Lab

Credit: 02
(Lab: 60 Hours)

A. Synthesis of Nanomaterials

1. Synthesis of Nanomaterials by Solid-state /Sol-gel method/Co-precipitation /combustion method
   a) TiO_2
   b) ZnO
   c) CdS
   d) Fe_2O_3/Fe_3O_4

2. Synthesis and characterization of core-shell nanocomposite (bimetallic and oxides)
3. Nanochemistry of silver nanoparticles in converting *p*-nitrophenol to *p*-aminophenol.
4. Synthesis of Graphene oxide nanopowder
5. Synthesis of Carbon nano tube

B. Applications

a) Catalytic study of synthesized materials through UV-VIS spectrophotometry
b) Other characterization facility available in the Department (XRD, FTIR, TEM, SEM etc.)

Reference Books:

- Pradeep, T. *A Textbook of Nanoscience and Nanotechnology*, McGraw Hill Edu. New Delhi, (2015).
- G. L. Hornyak, J. J. Moore, H. F. Tibbals, and J. Dutta: *Fundamentals of Nanotechnology*, CRC Press, 2009

CHM T 805: Polymer Chemistry

Credits: Theory-04
Theory: 60 Hours

Unit – 1: Introduction

Importance of polymers. Basic Concept: monomers, repeat units, degree of polymerization; linear, branched, and network polymers; classification of polymers. Polymerization: condensation, addition, radical, chain- ionic- and co-ordination-, and co-polymerization; polymerization condition and polymer reaction; polymerization in homogeneous and heterogeneous systems.

(12 Hours)

Unit– 2: Polymer Characterization Techniques

Polydispersion-average molecular weight concept; number, weight and viscosity average molecular weights. Polydiversity and molecular weight distribution. The practical significance of molecular weight. Measurement of molecular weights. End group, viscosity, light scattering, osmotic, and ultracentrifugation methods. Analysis and testing of polymers-chemical analysis of polymers. Spectroscopic methods, X-ray diffraction, microscopy studies. Thermal analysis and physical testing tensile strength, fatigue, impact, tear resistance, hardness and abrasion resistance analysis.

(12 Hours)

Unit – 3: Structure and Properties

Morphology and order in crystalline polymers – configuration of polymer chains; crystal structure of polymers; morphology of crystalline polymers; strain-induced morphology; crystallization and melting polymer structure and physical properties – crystalline melting point, T_m, melting points of homogeneous series effect of chain flexibility and other steric factors, entropy and heat of fusion. The glass transition temperature, T_g, relationship between T_m and T_g, effect of molecular weight, diluents, chemical structure, chain topology, branching and cross linking. Properties requirements for polymer utilization.

(12 Hours)

Unit – 4: Polymer Processing

Plastic, elastomers and fibres, compounding; processing techniques- calendaring, die casting, rotational casting, film casting, injection casting, blow moulding, extraction moulding, thermoforming, foaming, reinforcing, and fibre spinning.

(12 Hours)

Unit – 5: Properties of Commercial Polymers

Polyethylene, polyvinyl chloride, polyamide, polyester, phenolic resins, epoxy resins and silicone polymers. Functional polymers – fire retarding polymers and electrically conducting polymers. Biomedical polymers – contact lens, dental polymers, artificial heart, kidney, skin, and blood cells.

(12 Hours)

Reference Books:

- Fred W. Billmeyer: *Textbook of Polymer Science*, Eds: 3rd, Wiley-India, New Delhi, 2012.
- A Ravve: *Principle of Polymer Chemistry*, Eds. 3rd, Springer Science + Business Media, New York, 2012.
- J. M. G. Cowie: *Physics and Chemistry of Polymers*, Blackie Academic and Professional.
- H. R. Alcock and F. W. Iamtee: *Contemporary Polymer Chemistry*, Prentice Hall.
- V. R. Govarikar, N. V. Viswanathan, and J. sreedhar: *Polymer Science*, Wieley-Eastern.

CHM P 805: Polymer Chemistry Lab

Credit: 02
(Lab: 60 Hours)

1. Polymer Synthesis:

i) Free radical solution polymerization of styrene (St) / Methyl Methacrylate (MMA) / Methyl Acrylate (MA) / Acrylic acid (AA).
Purification of monomer
Polymerization using benzoyl peroxide (BPO) / 2,2'-azo-bis-isobutylonitrile (AIBN)

ii) Preparation of nylon 66/6
iii) Redox polymerization of acrylamide
iv) Precipitation polymerization of acrylonitrile
v) Preparation of urea-formaldehyde resin
vi) Preparations of novalac resin/resold resin.

2. Polymer characterization

i) Determination of molecular weight by viscometry:
Polyacrylamide-aq.$NaNO_2$ solution
ii) Determination of the viscosity-average molecular weight of poly(vinyl alcohol) (PVOH) and the fraction of "head-to-head" monomer linkages in the polymer.
iii) Determination of molecular weight by end group analysis: Polyethylene glycol (PEG) (OH group).

3. **Polymer analysis**

i) Estimation of the amount of HCHO in the given solution by sodium sulphite method
ii) Instrumental Techniques
iii) IR studies of polymers
iv) DSC analysis of polymers
v) Preparation of polyacrylamide and its electrophoresis

*at least 5 experiments to be carried out along with possible characterization.

Reference Books:

- Malcohm P. Stevens, Polymer Chemistry: An Introduction, 3rd Ed.
- Harry R. Allcock, Frederick W. Lampe and James E. Mark, Contemporary Polymer Chemistry, 3rd ed. Prentice-Hall (2003)
- Fred W. Billmeyer, Textbook of Polymer Science, 3rd ed. Wiley-Interscience (1984)
- Joel R. Fried, Polymer Science and Technology, 2nd ed. Prentice-Hall (2003)
- Petr Munk and Tejraj M. Aminabhavi, Introduction to Macromolecular Science, 2nd ed. John Wiley & Sons (2002)
- L. H. Sperling, Introduction to Physical Polymer Science, 4th ed. John Wiley & Sons (2005)
- Malcolm P. Stevens, Polymer Chemistry: An Introduction, 3rd ed. Oxford University Press (2005)
- Seymour/ Carraher's Polymer Chemistry, 9th ed. by Charles E. Carraher, Jr. (2013).

CHM T 806: Bioorganic and Drug Chemistry

Credits: Theory-04
Theory: 60 Hours

Unit – 1: Overview of Bioorganic Chemistry

***Introduction*:** Definition of bioorganic chemistry, Border line of bioorganic chemistry and inter disciplinary area between chemical and biology, Weak interaction in organic and biological world, Molecular Recognition.

***Chemistry of the Living Cell*:** The structure of prokaryotic and Eukaryotic cells, Composition of living cells:

(12 Hours)

Unit – 2: Carbohydrates, Proteins, Lipids, and Nucleic Acids

***Carbohydrates*:** Introduction, Reactions of Monosaccharides, Interconversions, Ring structure of aldoses and ketoses, Confirmation of Monosaccharides, Disaccharides: Structure, synthesis and properties.

***Proteins*:** General structure & classification of amino acids, Abbreviation of amino acids, Essential and non essential amino acids, Synthesis of amino acids, Isoelectric point, Acid and base properties of amino acids. Protein: Naturally occurring peptides, Modern methods of peptide synthesis with protection and deprotection, Determination of sequences and basic units of a poly peptides or proteins, C- & N-terminus detection by chemical methods, Primary, secondary, tertiary and quaternary structures of proteins, Enzyme active sites, allosteric sites, and mechanism of their actions e.g. chymotrypsin, carboxypeptidase, lipases etc.

***Lipids*:** Lipid structure- acylglycerols, phosphoglycerides and sphingolipids, Biological importance of fatty acids and lipids, Bio- and chemical Synthesis of lipids.

***Nucleic Acids*:** Definition, structure and properties, base pairing, double helices, Genetic information storage, transmission and gene expression, Nucleotides and Nucleosides: Similarities and differentiation, Structure of DNA & RNA. Types of mRNA, tRNA and rRNA, Replication, transcription and translation, Genetic code, Protein biosynthesis.

(16 Hours)

Unit – 3: Analogy Between Biochemical and Organic reactions

Introduction to metabolism (catabolism, anabolism). ATP: The universal currency of cellular energy, ATP hydrolysis and free energy change. Agents for transfer of electrons in biological redox systems: NAD^+, FAD. Conversion of food to energy: Outline of catabolic pathways of carbohydrate- glycolysis, fermentation, Krebs cycle. Overview of catabolic pathways of fat and protein. Interrelationship in the metabolic pathways of protein, fat and carbohydrate. Caloric value of food, standard caloric content of food types.

(10 Hours)

Unit – 4: Overview of Drug Chemistry and Basics of Drug Action

Definition, classification and nomenclature of drugs, Preliminary idea of drug action: Interaction (Weak interaction in drug molecules, Chirality and drug action), Receptorology (Drug-receptor interactions, Enzyme kinetics in drug action, Enzyme inhibitors (Drug action through enzyme inhibition), Nucleic acids as targets for drug actions, NA-Alkylation, NA-strand breaking and their importance in drug action, Drug metabolism, drug deactivation and elimination.

(12 Hours)

Unit – 5: Pharmaceutical Compounds: Structure and Importance

Classification, structure and therapeutic uses of antipyretics: Paracetamol (with synthesis), Analgesics: Ibuprofen (with synthesis), Antimalarials: Chloroquine (with synthesis). An elementary treatment of Antibiotics and detailed study of chloramphenicol, Medicinal values of curcumin (haldi), azadirachtin (neem), vitamin C and antacid (ranitidine).

(10 Hours)

Reference Books:

- L. Stryer: *Biochemistry*, 4th Edition W. H. Freeman and Co. 1995.
- S. Zubay: *Biochemistry*, Addison-Wesely 1983.
- J. Mann; R.S. Davidson: *Natural Products: Chemistry and Biological Significance*
- H. Dugas: *Bioorganic Chemistry Frontiers Vol. 2*, ed. Springer-Verlag, 1990.
- E. E. Tamlen: *Bioorganic Chemistry*, Academic Press, 1977.
- M. Bodansky: *Peptide Chemistry: A Practical Textbook*, Springer-Verlag 1988.
- *Bioorganic Chemistry: A chemical approch to enzyme action*, Springer-Verlag 1989.
- W. Saenger: *Principles of Nucleic acid structures*, Springer-Verlag 1984.
- G. R. Chatwal: *Medicinal Chemistry*
- A. Kar: *Medicinal Chemistry*, Wiley, 2000.
- D. Lednicer: *Strategies for Organic Drug Synthesis and Design*, John Wiley 1998.
- G. R. Chatwal: *Synthetic Drugs*, Himalaya, New Delhi 1995.
- S. Hanessian, *Total synthesis of Natural product: The chiral approach Vol.III* Pergamon Press 1983.
- W. D. Foye, T. L. Lemke, and D. A. Williams: *Principles of Medicinal Chemistry (*4th Edition)
- R. B. Siwerman: *Organic Chemistry of Drug Action and Design* (Academic press, 1993).

CHM P 806: Bioorganic and Drug Chemistry Lab

Credits: 02
(Lab: 60 Hours)

(a) Synthesis of Following Drug Molecules:

1. Paracetamol,
2. Acetanilide,
3. Aspirin,
4. Phenazone
5. Ibuprofen

(b) Synthesis of short peptide containing 2-3 different amino acids.

(c) Crararacterization:

1. Practices for recording the UV-visible spectra of suitable chromophoric molecules.
2. Sample preparation and recording the IR Spectra for IR-active compounds.
3. Analyze the first-order/ second order ^{1}H-NMR Spectra of any standard organic molecules (Identification of chemical shifts for all protons, measurement of coupling constant, diastereoisomers ratio, determination of chemical yields by using a standard)
4. Analyze the 2D-^{13}C-NMR spectra of any organic molecules.
5. Analytical separation of diastereoisomers and enantioisomers by using HPLC techniques and determining the enantiomeric purity (ee/er) and diastereoisomers ratio (d.r.) by HPLC chromatogram.

After completion of above hands on experiences, a student would be enabling to analyze any unknown spectroscopic datas (e.g.; UV-Visible spectra, IR Spectra, 1H-NMR spectra and 13C-NMR Spectra).

References of Books:

- Khosla, B. D.; Garg, V. C. & Gulati, A., *Senior Practical Physical Chemistry*, R. Chand & Co.: New Delhi (2011).
- Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. *Experiments in Physical Chemistry 8th Ed.;* McGraw-Hill: New York (2003).
- Halpern, A. M. & McBane, G. C. *Experimental Physical Chemistry 3rd Ed.;* W.H. Freeman & Co.: New York (2003).
- Bessler and Silverstein, Spectroscopy of Organic Compounds, JOHN WILEY, 2001.
- D. C. Pavia, G. M. Lampman, G. S. Kriz, Introduction to Spectroscopy, *3*rd *Edition*, THOMSON, 2007.
- Organic Spectroscopy III Edition–by William Kemp

CHM T 807: Advanced Heterocyclic Chemistry

Credits: Theory-04
Theory: 60 Hours

Unit – 1: Introduction

Definition of heteroatom, Aromatic and non-aromatic heterocyclic compounds, Classification and nomenclature of heterocyclic compounds, important reactions with heterocyclic compounds i.e. oxidation, reduction and tertiary effect of Nitrogen in heterocyclic compound.

(12 Hours)

Unit – 2: Non-Aromatic Heterocycles

Different types of strains, interactions and conformational aspects of non-aromatic heterocycles. Synthesis, reactivity and importance of the following ring systems: Aziridines, Oxiranes, Thiiranes, Oxaziridines, Azetidines, Oxetanes and Thietanes.

(12 Hours)

Unit – 3: Five and Six Membered Heterocyclics with One Hetero Atom

Pyrrole, Furan, Thiophene, Pyridine, Indole, Quinoline, Isoquinoline - Synthesis and reactions [Advanced level Synthetic preparation or method applied].

(12 Hours)

Unit – 4: Five and Six Membered Heterocyclics with Two Hetero Atoms

Synthesis, reactivity, aromatic character and importance of the following heterocycles: Pyrazole, Imidazole, Oxazole, Thiazole, Isoxazole, Isothiazole, Pyridazine, Pyrimidine. Pyrazine, Oxazine, thiazine, benzimidazole, benzoxazole and benzthiazole.

(12 Hours)

Unit – 5: Larger Ring and Other Heterocycles

Synthesis, structure, stability and reactivity of Azepines, Oxepines and Thiepines. Synthesis of Benzoazepines, Benzooxepines, Benzothiepines, Azocines and Azonines.

(12 Hours)

Reference Books:

- T. Gilchrist: *Heterocyclic Chemistry*
- R. M. Acheson: *An Introduction to the Chemistry of Heterocyclic Compounds*
- J. A. Joule & K. Mills: *Heterocyclic Chemistry*
- A. Paquette: *Principles of Modern Heterocyclic Chemistry*
- J, A. Joule & Smith: *Heterocyclic Chemistry*
- A .R. Katritzky: *Handbook of Heterocyclic Chemistry*

CHM P 807: Advanced Heterocyclic Chemistry Lab

Credits: 02
(Lab: 60 Hours)

1. Three member Heterocycles:

i) Epoxide synthesis from alkenes
ii) Epoxide synthesis from Halohydrin substrates
iii) Aziridination of alkenes
iv) Aziridine synthesis from amino acids

2. Five member Heterocycles:

i) Hantzsch synthesis of Pyrrole.
ii) Multicomponent reaction for synthesis of Pyrrole (Jana method).
iii) Meyer's Oxazoline synthesis from amino alcohol.

3. Fused five- or six member heterocycles:

i) Indole synthesis
ii) Quinoline synthesis
iii) Synthesis of 1-Phenyl-1,2,3,4-tetrahydroisoquinolines.

4. Basic reactions with heterocycles:

a) Treatment of Br_2 in MeOH and followed by oxidation with Amberlyst-15.
b) [3+2]-cycloaddition reaction of aziridine and carbonyl compounds in the presence of Lewid acid.

References of Books:

- *Practical Organic Chemistry* by A. I. Vogel.
- *Practical Organic Chemistry* by F. G. Mann and B. C. Saunders.
- The Organic Chemistry Journals: plz search Supporting informations of Journal of Organic chemistry, Organic Letters and Journal of American chemical Society from ACS Publication and Angew. Chem. Int. Ed. (Willey publishers); Chemical Communication (Royal Chemical Society) for appropriate experimental methods.
- *Journal of Chemical Education* **1985**, *62*, 262.

CHM T 808: Chemistry of Natural Products

Credits: Theory-04
Theory: 60 Hours

Unit – 1: Alkaloid – I

Occurrence and isolation, biological role of alkaloids, General properties, nomenclature and classification of alkaloids on the basis of amino acid origin and present core structure. Isolation, properties and structural elucidation of quinine, Morphine (structure, synthesis, molecular rearrangement, stereochemistry and biogenesis).

(12 Hours)

Unit – 2: Alkaloid – II

Structure and biological role of nicotine, cocaine, quinine, reserpine, vincristine, morphine, caffeine, papavarine, hyocimine. Strychnine and lysergic acid.

(12 Hours)

Unit – 3: Steroid

Introduction, nomenclature of steroids, absolute configuration of steroid. Occurrence, isolation, structute elucidation and chemical properties of Cholesterol.

(12 Hours)

Unit – 4: Terpenes

Secondary metabolites: Definition and examples; terpenes – isoprene rule; mono terpenes: structure of geraneol, limonene, alpha-pinene and camphor; sesquiterpenes: longfolene;

diterpenes: abietic acid, taxol. Structure determination of Citral and Camphor.

(12 Hours)

Unit – 5: Vitamins

Introduction, chemical properties, structure elucidation of Vitamin A, Vitamin B, Ascorbic Acid and Vitamin D. Vitamin A and its role in vision. Biological role of Vitamin D, Ascorbic Acid, Vitamin A.

(12 Hours)

Reference Books:

- I. L. Finar: *Organic Chemistry Vol. II*, 5th Edition
- S. V. Bhat, B. A. Nagaramgagi, M. Srikumar: *Chemistry of Natural Products*, Alpa Science International Ltd, 2005 by
- O. P. Agarwal: *Chemistry of Natural Products, Vol I & Vol II*, Goel publishing House, 1989
- J. R. Hanson: *Natural Products: The Secondary Metabolites*, Wiley-Vch, 1st Ed.

CHM P 808: Chemistry of Natural Products Lab

Credits: 02
(Lab: 60 Hours)

Extraction

1. Extraction of caffeine from tea leaves.
2. Lycopene extraction form Tomatoes
3. Extraction of DNA from onion/cauliflower
4. Separation of amino acids by paper chromatography
5. Study of titration curve of glycine
6. To determine the saponification value of an oil/fat.
7. To determine the iodine value of an oil/fat
8. Practical Synthesis of of any one indole alkaloids.
9. If possible, extraction of any alkaloids from plants.

References:

- Furniss, B.S.; Hannaford, A.J.; Rogers, V.; Smith, P.W.G.; Tatchell, A.R. *Vogel's Textbook of Practical Organic Chemistry*, ELBS.
- Ahluwalia, V.K. & Aggarwal, R. *Comprehensive Practical Organic Chemistry,* Universities Press.
- Journal of Chemical Education, **2008**, *85*, 256.

CHM T 809: Advanced Synthetic Organic Chemistry

Credits: Theory-04
Theory: 60 Hours

Unit – 1: Metal Mediated C-C and C-X Coupling Reactions

Suzuki, Heck, Stille, Sonogishira cross coupling, Buchwald-Hartwig and Negishi-Kumada coupling reactions. **C=C Formation Reactions:** Shapiro, Bamford-Stevens, McMurrey reactions, Julia Lythgoe olefination and Peterson's stereoselective olefination. Olefin metathesis by I^{st} and II^{nd} generation catalysts: Reaction mechanism and application in the synthesis of heterocycles.

(12 Hours)

Unit– 2: Reagents of Phosphorous, Sulfur, Silicon and Boron

Phosphorous Sulfur, Silicon and Boron containing compounds-preparations and their uses in organic reactions.

(12 Hours)

Unit – 3: Oxidation and Reduction

***Oxidation*:** Oxidation of hydrocarbons (alkanes, aromatic hydrocarbons, alkenes), Oxidation of alcohols (Chromium reagents, Manganese reagents, Other metal and non-metal based oxidants), Oxidation of ketones (α, β-unsaturated ketones, α-hydroxy ketones, Baeyer-Villiger oxidation of ketone)

***Reduction*:** Catalytic hydrogenation, Reduction by dissolving metals, Reduction by hydride-transfer reagents (Derivatives of lithium aluminium hydride and sodiumborohydride, mixed lithium aluminium hydride-aluminium chloride reagent, DIBAL-H, $NaBH_3CN$, sodium triacetoxyborohydride, Borane and derivatives, other methods of reductions).

(12 Hours)

Unit – 4: Disconnection Approach, Umpolung Chemistry and Protection-Deprotection of Functional groups

Basic principles and terminology-Target molecule, FGI, Disconnection, Synthon, Reagent and Retro-synthetic approach. **One group C-C and C-X disconnection**: (disconnection of alcohols, alkenes, and carbonyl compounds). **Two group C-C & C-X disconnections**: 1,3 and 1,5 difunctionalised compounds, α, β, unsaturated carbonyl compounds, control in carbonyl condensation, synthesis of 3,4,5 and 6 membered rings in organic synthesis. Diels-Alder reaction, connection in retro synthesis. Umpolung in organic synthesis. Protection and deprotection for functional groups as hydroxyl, amino, carboxylic and carbonyl.

(12 Hours)

Unit – 5: Some Important Organic Reactions

Selective Stereoselective Organic Reactions with Alkenes: Sharpless Asymmetric Epoxidation, Asymmetric Aziridination, Dihydroxylation, Amino-hydroxylation Reactions, Oxidative cleavages of alkenes.

Green Chemistry, Supramolecular chemistry (Crown ether, Cyclodextrin and Clalixerins) and multicomponent reactions (Ugi, Passerini, Biginelli, Hantzsch reactions).

***Chemistry of Aliphatic and Aromatic Heterocyclic Compounds*:** Epoxide, Aziridine, Azitidine, Oxetane, Pyrrole, Furan, Thiophene, Pyridine, Indole, Quinoline, Isoquinoline - Synthesis and reactions.

(12 Hours)

References Books:

- B. F. G. Johnson: *Transition Metal Cluster*, Wiley, 1980.
- R. H. Crabtree: *The Organometallic Chemistry of the Transition Metals*, Wiley-Interscience, 2005.
- G. Wikinson, F. G. A. Stone, and E. Abel: *Comprehensive Organometallic Chemistry*, Peramon, 1980.
- I. Fleming: *Frontier Orbitals and Organic Chemical Reactions*, Wiley, 1976.
- B. B. Woodward and Hoffman: *Conservation of Orbital Symmetry*, Verlag Chemie Academic Press, 1971.
- S. Warren: *Organic Synthesis: The Disconnection Approach*, John Wiley & Sons (Asia) Pte. Ltd., 2007
- W. Carruthers and I. Coldham: *Modern Methods of Organic Synthesis*, Fourth Ed. Cambridge University Press.
- T. L. Gilchrist: *Heterocyclic Chemistry*, Pearson Education, 3rd Ed.2007

CHM P 809: Advanced Synthetic Organic Chemistry Lab

Credits: -02
Lab: 60 Hours

1. Pd-catalyzed Heck reaction (Reaction design, starting material preparation if not commercially available, reaction set-up, monitoring the reaction progress, purification and spectroscopic analysis should be carried out by each student).

2. Pd-catalyzed Suzuki coupling reaction (Reaction design, starting material preparation if not commercially available, reaction set-up, monitoring the reaction progress, purification and spectroscopic analysis should be carried out by each student).

3. Pd-catalyzed Sonogishira coupling reaction (Reaction design, starting material preparation if not commercially available, reaction set-up, monitoring the reaction progress, purification and spectroscopic analysis should be carried out by each student).

4. Wittig reaction and Wittig Horner method for alkene synthesis (Any one suitable example from each reaction).

5. Oxidation and Reduction (choose any one suitable example from each category)
   (i) Oxidation of secondary alcohol to ketone
   (ii) Oxidation of primary alcohol to aldehyde
   (iii) Reduction of aldehydes by $NaBH_4$
   (iv) Reduction of ketones by $LiAlH_4$

6. Synthesis of an Imidazolidinone Organocatalyst and its application in a DA Reaction: Multistep Synthesis
   (i) Catalyst synthesis
   (ii) Diels-Alder reaction.
   (iii) Purification step
   (iv) Spectral data analysis (1H-NMR and 13C-NMR)

7. Multi component reaction: Biginelli reaction

References Books:

- *Practical Organic Chemistry* by A. I. Vogel.
- *Practical Organic Chemistry* by F. G. Mann and B. C. Saunders.
- For Pd-catalyzed cross coupling reaction, recommend ACS journal's Supporting Information
- *J. Chem. Edu.* (DOI: 10.1021/acs.jchemed.5b00812)
- *Advanced Practical Organic Chemistry* by J. Leonard, B. Lygo and G. Proctor.

CHM T 810: Principles of X-ray Diffraction and Electron Microscope

Credits: Theory-05, Tutorial: 01
Theory: 75 Hours

Unit – 1: Geometry of Crystal Structure

Form of solids, space lattice, seven crystal systems; unit cell, primitive and non-primitive cell,, Bravais lattice, lattice direction and crystal planes; Miller indices of crystal planes, separation between crystal planes, reciprocal lattice

Crystal Structure; closed packed structure- hcp and ccp, rack salt (NaCl), Wurzite and zinc blend of ZnS, diamond, CsCl, Fluoride (CaF_2) and antifluoride (Na_2O), Rutile (TiO_2) *etc*.

(15 Hours)

Unit – 2: Point and Space Groups

Symmetry operation and symmetry elements, Plane of symmetry, inversion centre, proper and improper axis of rotation, product of symmetry operation, Relation among symmetry elements and symmetry operation, thirty two point groups, representation of point groups with selected examples like 222, mm2, mmm, 32 centrosymmetric and non-centrosymmetric point groups.

Space group: Triclinic P1, monoclinic C2, monoclinic C2/m, orthorhombic $P222_1$ orthorhombic F222, Tetragonal 14_1, space group and crystal structure of perovskite ABO_3 and rutile structure of TiO_2 etc

(15 Hours)

Unit – 3: X-ray Diffraction by Crystal

Properties of X-rays, production and detection of X-ray, diffraction of X-ray by crystal, Bragg's condition, Brag's law, diffractometer and diffractometer methods (Laue, rotating-crystal, and powder methods), Scherrer formula, scattering of an electron, atom, by a unit cell, structure factor, systematic absence, intensity of powder pattern line.

Determination of crystal structure, chemical analysis by X-ray diffraction, chemical analysis by X-ray spectroscopy (EDX energy dispersive X-ray spectroscopy).

(15 Hours)

Unit – 4: Electron Microscope

Introduction: optical microscope versus electron microscopy, brief history of electron microscope, interaction of electron and matter, elastic in-elastic scattering of electron,

Instrument: scanning electron microscope (SEM), transmission electron microscope (TEM); electron source; lenses and lenses defects, apertures and resolution, electron detection and display, pumps and sample holders, calibration of imaging system, specimen preparation for TEM

(15 Hours)

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Unit – 5: Transmission Electron Microscope

Forming diffraction pattern and images; principle of image contrast, bright field and dark field imaginings, and SAED and obtaining SAED, high-resolution TEM, grain boundary, phase boundary, and other imaging techniques.

Reciprocal space; diffraction from crystals; diffraction from particles, and dislocation, indexing of diffraction patterns, Kikuchi diffraction.

(15 Hours)

References Books:

- A. R. West: *Solid State Chemistry and Its Applications*, John Wiley & Sons, 1989.
- L. Smart and E. Moore, *Solid State Chemistry*, Chapman and Hall, 1992.
- A. K. Cheetham and P. Day: *Solid State Chemistry Compounds*, Clarendon Press, Oxford 1992.
- C. N. R. Rao and J. Gopalkrishanan: *New Directions in Solid State Chemistry*, Cambridge Univ. Press 1997.
- D. B. Williams and C. B. Carter: *Transmission Electron Microscopy: A Textbook for Materials Science*, Plenum Press, New York, 1996.
- B. D. Cullity: *Elements of X-ray Diffraction*, Eds: 2nd, Addison-Wesley, USA, 1959.

Tutorials: **Credit: 01**

- **Indexing and calculating of powder XRD pattern for cubic and non-cubic system.**
- **Indexing of SAED pattern and quantifying and processing of TEM, HRTEM images.**

References Books:

- D. B. Williams and C. B. Carter: *Transmission Electron Microscopy: A Textbook for Materials Science*, Plenum Press, New York, 1996.
- B. D. Cullity: *Elements of X-ray Diffraction*, Eds: 2nd, Addison-Wesley, USA, 1959.