SYLLABUS OF PRE-REGISTRATION COURSE WORK (ONE SEMESTER) FOR THE Ph.D. PROGRAMME IN CHEMISTRY

DIBRUGARH UNIVERSITY

Approved by BOS in Chemistry held on 14.12.2018

DISTRIBUTION OF MARKS OF THE COURSE WORKS:

No. / Code	Total	Credit	Internal Assessment	End Semester Examination
Course – I	100	4	40	60
Course - II	100	4	40	60
Course-III	100	4	40	60
Course-IV	100	4	80 (assignment writing)	20 (viva on the assignment)

Total Marks: 400; Total Credit : 16

1. Candidates shall have to secure a minimum of 45% of marks in aggregate to pass a paper individually.

2. There shall be internal assessment of 40 marks in each theory paper to be awarded against the following:

Sessional Exam I	15 Marks
Sessional Exam II	15 Marks
Seminar Presentation etc	10 Marks

Ph.D. Course Work
Course-I
Research Methodology
60 + 40 (Internal Assessment) =100

Unit-I **Marks 25**

Basics of research methodology:

Information survey, Sources of information, data collection, processing and tabulation, effective writing, Scientific and technical report writing. Statistical analysis of data. Objective, methodology including tools of analysis to be used, proposed sources of data, characterization; Scientific work place, importance of impact factors, citation index of publication. Writing a grant proposal (in prescribed format of DST, DBT, CSIR, UGC, etc.)

Unit-II: **Marks:25**

Separation and Characterization techniques:

Problems relating to structural analysis of chemical compounds and materials using IR, UV-VIS, NMR, ESR and Mass spectroscopy; SEM-EDX, TEM, XRD (Powder and single crystal); Chromatographic techniques, GC-MS, LC-MS; Thermal analysis (TGA, DTA, DSC).

Unit-III **Marks: 10**

Intellectual Property Rights (IPR):

Introduction of Intellectual Property; Different components of IPR: Patent, Copyright, Geographical Indications, Trademarks, Industrial Design; Information related to: Patent search, drafting and filing (India as well as Foreign).

Books Recommended:

General Spectroscopy

1. Vibrational Spectroscopy – Theory and Application. D.N. Sathyanarayana, New Age Publication.
2. Fundamentals of Molecular Spectroscopy: Colin N. Banwell and Elaine M. McCash, Tata McGraw Hill
3. Spectroscopic Methods in Organic Chemistry: D.H. Williams and Ian Fleming, Tata-McGraw Hill
4. Spectrometric Identification of Organic Compounds: R.M. Silverstein, G.C. Bassler and T.W. Morril, John Wiley and Sons

General Physical Methods

1. Physical Methods for Chemists: R.S. Drago, Saunders College Publishing
2. Structural Methods in Inorganic Chemistry: E.A.V.D. Ebsworth, D.W. H. Rankin and S. Cradock, Blackwell
3. Principles and Practice of Analytical Chemistry: F.W.Fifield and D. Kealey, Blackie Academic and Professional
4. Analytical Chemistry: G.D. Christian, John Wiley and Sons

5. Analytical Chemistry: Principles: J.H. Kennedy, Saunders College Publishing
6. Undergraduate Instrumental Analysis: J.W. Robinson, Marcel Dekker

NMR Spectroscopy

1. Nuclear Magnetic Resonance Spectroscopy: F.A. Bovey, Academic Press
2. NMR in Chemistry: A Multinuclear Introduction: William kemp, Macmillan
3. Structure Elucidation by NMR in Organic Chemistry: E. Breitmaier, Wiley
4. Modern NMR Techniques for Chemistry Research: A.E. Derome, Pergamon Press
5. NMR Spectroscopy, Basic Principles, Concepts and Applications in Chemistry: H. Gunther, John Wiley and Sons

Electronic Spectroscopy

1. Inorganic Electronic Spectroscopy: A.B.P. Lever, Elsevier science Publishers
2. Theory of Electronic Spectra of Organic Molecules: J.N. Murrel,

Vibrational Spectroscopy

1. Vibrational Spectroscopy: Volume I and II: Nakamoto

Application of Spectroscopic methods in problem solving

1. Organic structures from spectra, S. Sternhell & J.R. Kalman, John Wiley & sons.
2. NMR spectra catalogue (Aldrich) Vol.-I, II, III.

Thermal Methods

1. Principles and Applications of thermal analysis: P.J. Haines.

Intellectual Property Rights (IPR:

Online WIPO document:

http://www.wipo.int/edocs/pubdocs/en/intproperty/450/wipo_pub_450.pdf

www.uspto.gov/

Ph.D. Course Work
Paper – II
Inorganic Chemistry (optional)
Marks 60 + 40 (Int. Ass) = 100

Unit – I: Marks-25

Co-ordination Compounds: MO theory of transition metal complexes, Electronic spectra of d^1-d^9 complexes, Magnetic properties of transition metal complexes. Distortion from octahedral symmetry - Jahn Teller Effect. Angular overlap model (qualitative aspect only).

Main group and transition metal (1^{st} and 2^{nd} row) organometallics, metal carbon σ and π bonded compounds. MO description of organometallic compounds of alkene, alkyne, allyl, butadiene, cyclobutadiene and arene metal compounds. Fluxional behaviour and catalysis by organometallic compounds. Transition metal and main group compounds showing supramolecular interaction.

Unit - II: Marks – 20

Bioinorganic and macrocyclic Chemistry: Bioinorganic Chemistry of Fe, synthetic blood, Iron-sulfur proteins, cytochromes, vitamin B_{12}, nitrogenase, hydrogenase and copper oxidase. Crown ethers, cryptands of alkali and alkaline earths, Metal complexes as antioxidants.

Unit-III: Marks-15

Inorganic reaction mechanism: Stability constant; lability and inertness; mechanism of ligand replacement reaction; substitution reaction in octahedral and square planner complex; trans effect and its applications; hydrolysis reactions; isomerization and racemisation reactions; electron transfer reactions; Inner sphere and outer sphere mechanisms; template reactions.

1. Bioinorganic Chemistry by K. Hussain Reddy, New Age International Publisher.
2. The Inorganic Chemistry of Biological Processes, Hughes, M.N., 2^{nd} edition, Wiley (1981)
3. Bio-coordination Chemistry, D.E. Fenton, Oxford University Monograph Series 1995.
4. Inorganic Chemistry, Shriver & Atkins, 5^{th} Edition Oxford
5. Inorganic Chemistry Principles and Structure –J. E. Huheey

Ph. D. Course work
Paper II: Organic Chemistry (Optional)
Marks 60 + 40 (Int. Ass) = 100

Unit I: Spectroscopic Techniques in Organic Chemistry Marks 20

NMR: Chemical shifts and factors influencing the chemical shift, Spin-spin coupling, Spin decoupling, Shift reagent, NOE, ^{13}C, ^{15}N, ^{19}F and ^{31}P, COSY, NOESY, 2D NMR,

Use of IR in structure elucidation,

General principles and utilization of Mass spectrometry, fragmentation patterns of different organic compounds.

Books Recommended:

1. Fundamentals of Molecular spectroscopy, Colin N. Banwell and Elaine M. McCash, Tata McGraw Hill
2. Spectroscopic methods in Organic Chemistry: D.H. Williams and Ian Fleming, Tata McGraw Hill
3. Spectroscopic identification of Organic Compounds: R. M. Silverstein, G.C. Bessler and T.W. Morril. John Wiley and Sons.
4. Vibrational Spectroscopy, Volume I and II, Nakamoto.
5. NMR in Chemistry, A Multinuclear Introduction, William Kemp, Macmillan

Unit II: New reagents for Organic Synthesis Marks 20

Organo-transition metal reagents: Use of transition metals at different oxidation states in organic synthesis (Ti, Cr, Fe, Ru, Rh, Ni, and Cu), Olefin Metathesis reaction (Grubb's catalyst), Ziegler Natta catalyst.

Phosphorus, Sulfur and Nitrogen ylides: Preparation, applications in organic synthesis and mechanism.

Umpolung in organic synthesis.

Protection and deprotection of hydroxyl, amino, carboxyl, ketone and aldehyde functions with special reference to the synthesis of polypeptide and polynucleotide. Solid phase peptide synthesis

Books Recommended:

1. Organic Chemistry – Paula Yurkanis Bruice, Pearson
2. Organic Chemistry- Clayden, Greeves, Warren and Wothers, Oxford University Press.
3. Advanced Organic Chemistry Part A and B : Carey and Sundberg
4. Modern Methods of Organic Synthesis – Carruthers and Mendham, Cambridge University Press
5. Organic Synthesis – M.B. Smith, McGraw Hill. (Reference book)
6. Principles of Organic Synthesis – R.O.C. Norman and J M Coxon
7. Organic Synthesis : M.B. Smith, Tata McGraw Hill

8. Advanced Organic Chemistry: Reactions, Mechanisms and Structure By J. March, Wiley
9. Organic Synthesis - Concepts, Methods and Starting Materials By J. Fuhrhop and G. Penzilin, Verlag VCH

Unit III: Stereochemistry of Pericyclic reactions Marks-20

Classification of stereoselective synthesis: diastereoselective and enantioselective reactions. Enantioselective synthesis – Use of chiral reagent, chiral catalyst and chiral auxillary. Conformational analysis of disubstituted cyclohexanes, cyclohexene, cyclohexanone. Stereoselectivity and regioselectivity of pericyclic reactions. Symmetry controlled reactions: Sigmatropic rearrangement – [m+n] sigmatropic shifts of hydrogen and carbon, Cope and Claisen rearrangement, Electrocyclic reactions, Click reactions.

1. Organic Chemistry- Clayden, Greeves, Warren and Wothers, Oxford University Press.
2. Advanced Organic Chemistry: Reactions, Mechanisms and Structure By J. March, Wiley.
3. Organic Chemistry – Paula Yurkanis Bruice, Pearson
4. Pericyclic Reactions- A Textbook by S. Sankararaman, Wiley
5. Frontier Orbitals and Organic Chemical Reaction – Ian Fleming, John Wiley

Ph. D. Course work
Paper II
Physical Chemistry (Optional)
Marks 60 + 40 (Int. Ass) = 100

(Any two Units will be taught)

Unit I: Polymer Chemistry **Marks 30**

Introduction to polymeric materials: Concept and definitions, polymer overview, classification of polymeric materials

Polymer reaction: Classification, addition polymerization, co-ordination polymerization, step polymerization, radical chain polymerization, chain polymerization kinetics, ionic polymerization, distinguishing between radical and ionic polymerization, group transfer polymerization, atom transfer radical polymerization, chain copolymerization, green polymerization techniques.

Polymer characterization Molecular weight of polymers: Molecular weight measurements – end group analysis, viscometry, get permeation chromatography, osmometry, light scattering, ultracentrifuge; practical significance of molecular weight; thermal analysis of polymers – thermal transitions of polymers; X-ray diffraction study of polymers; Instrumentation details of GPC, DSC, TGA, XRD on analysis of polymers; mechanical properties of polymers.

Polymer processing: Polymer in special use, high temperature and fire resistant polymers, liquid crystalline polymers, polymers, polyelectrolyies, biodegradable polymers, polymer composites, polyurethanes.

Unit II: Electrochemistry **Marks 30**

Electrical double layer, Thermodynamics and models, theory and instrumentation – Derivative Paleography, Ion selective electrodes – potentiometric titrations.

Electro catalysis: Electrocatalysis in simple redox reactions. The corrosion current and potential, Electrochemical energy conversion. High temperature fuel cells. Electronically Conducting organic polymers. Cyclic Voltammetry.

Unit III: Photochemistry **Marks 30**

Radiative and non-radiative transition of a photoexcited molecules; Photo physical kinetics of unimolecular processes; delayed fluorescence; effect of temp on emission processes; Concentration dependence of quenching and excimer foration;Quenching by foreign substances – exciplex foration; Electronic energy transfer mechanism of quenching; Photoxidation and photooxygenation; Photodimerisation.

Conversion and storage of solar energy; photoelectrochemical device for conversion of solar energy – photogalvanic cell.

Photochemistry in nature, atmospheric photochemistry in stratosphere and troposphere.

Unit IV: Solid State Chemistry **Marks 30**

Electrical conductivity, bonding in solid, band theory; Origin of Band Gap; Fermi dirac Statistics and Fermi energy; Motion of electrons in Bands and effective mass. Temperature dependence of Mobility, Temperatures variation of charge Carrier Densities.
Semi Conductors: Charge- Carrier Density in Intrinsic Semiconductor. Doping of Semi Conductors and its carrier devices. Super conductivity. BCS theory consequences of the BCS theory. Effect of Magnetic field. High temperature super conductors. Organic super conductors. Solid state reactions.

Unit V: Advanced Quantum Chemistry **Marks 30**

Review of vectors and vector spaces, matrices and determinants, eigenvalues and eigenvectors, Born-Oppenheimer approximation, Pauli Exclusion Principle, General rules for matrix element (with derivation), Second quantization, Electron correlation, Rayleigh-Ritz method, Restricted Closed-Shell and Unrestricted Open-Shell Hartree-Fock Methods, Introduction to Configuration Interaction, Rayleigh-Schrodinger Perturbation theory, and CC methods

Review of basic ideas of density functional theory, Hohenberg-Kohn theorems, Kohn-Sham formulation, review of the performance of the existing local and non-local density functionals.

Books Recommended:

Unit I:

1. G. Odian, “Principles of Polymerization”, Wiley & Sons, New York
2. F.W. Billmeyer, Jr. “Texbook of Polymer Science”, John wiley & Sons, New York
3. J.F. Rabek, “ Experimental Methods in Polymer Chemistry”, Wiley-Interscience, New York
4. “Comprehensive Polymer Science”, G. Allen, S.L. Aggarwal and S.Russo, Eds, Pergamon, Oxford.

Unit II:

1. Modern Electrochemistry – Vol 2A by John O’M Bockris, A.K.N. Reddy and Maria Gamboa – Aldeco.
2. Modern Electrochemistry – VI 2B J.O’M Bockris and A.K.U. Reddy.
3. Non-Aqueous Electrochemistry – by Doron Aurbach (Marcel Dekker, INC).

Unit III:

1. Fundamental of Photochemistry, K.K. Rohatgi – Mukherjee, Wiley-Eastern
2. Photochemistry – C.E. Wayne and R.P. Wayne, Oxford Science Publication
3. Introductory Photochemistry, A. Cox and T. Camp, McGraw Hill
4. Photochemistry – R.B. Cundall and A. Cox and T. Camp. McGraw Hill
5. Photochemistry – Culvert and Pitt
6. Essential of Molecular Photochemistry, A. Gilbert and J. Baggott, Blackwell Scientific publication
7. Molecular Photochemistry – N.J. Turro, W.A. Benzamin.

Unit IV:

1. Solid State Physics – An Introduction to principles of Material Science by Harald Ibach and Hans Liith – Springer – Publication – 2003.
2. Principles of the Solid State by H.V. Keer – New Age Intl. Publishers – 2005.
3. Introduction to Solids by L.V. azaroff.

Unit V:

1. Modern Quantum Theory – N.S. Ostlund and A. Szabo McGraw Hill.
2. Density functional theory of atoms and molecules, R.G. Parr and W. Yang, Oxford.
3. Methods of Molecular Quantum mechanics, R. McWeeney and B. T. Sutcliffe, Academic Press.

Ph. D. Course Work
Course-III
Symmetry and Group Theory (Optional)
Course Teacher: Prof. P. K. Gogoi
Marks 60 + 40 (Int. Ass) = 100

Unit-I: Marks-20

Symmetry operation, elements of symmetry: Matrices and matrix representation of symmetry operations, Definition of Group, finite and infinite group. Examples of groups using geometrical object and symmetry operations. Symmetry elements as elements of group. Point groups.

Unit II: Marks-20

Orthogonality theorem: reducible and irreducible representation, use of vectors and mathematical functions in group representation, Character table for molecular point group, construction of C_{2v} and C_{3v} Character table. Direct product representation. Projection operator, symmetry adapted linear combination (SALC) for C_{2v}, C_{3v}, D_{4h} and Td point group molecules.

Unit III: Marks-20

Chemical Application of Group Theory: Use of group theory in construction of hybrid Orbitals (d^2sp and sp^3 hybrids). Infrared absorption and Raman scattering spectroscopy, vibrational modes as bases for group representation, Symmetry selection rules for IR and Raman Spectra. Classification of vibrational modes and vibrational analysis. Orbital Symmetry and Chemical reactions –Woodward and Hoffman rules for electrocyclic and cycloaddition reactions.

Text books :

1. Chemical Applications of Group Theory by F.A. Cotton, Wiley Intersciences.
2. Symmetry and Spectroscopy of molecules K. Veera Reddy, New-Age International (P) Ltd. Publishers, Guwahati, 2005

Reference books:

1. Vibrational Spectroscopy by D.N. Sathyanarayana, New-Age International Publishers 2005
2. Introductory Group theory for Chemists by George Davidson, Elsevier Publishing Company Ltd., London.

Ph.D. Course Work
Course-III
Coordination Chemistry and Catalysis (Optional)
Course Teacher: Prof. Pankaj Das
Marks 60 + 40 (Int. Ass) = 100

Unit I: Characterization of metal complexes: 30

(i) NMR characterization: Basic principles, chemical shift, relaxation processes, NMR shift reagents, simplifications of complex spectra, characterization of metal complexes by NMR spectra (^{1}H, ^{13}C, ^{31}P, 19F), NMR spectra of paramagnetic molecules, applications of NMR in structure determination, NMR spectra of fluxional molecules. 20

(ii) IR and Mass spectra: Applications of IR and mass spectroscopy in characterizing metal complexes like carbonyl complexes, Schiff base complexes, etc. 10

Unit II: Catalysis 30

(i) Homogeneous catalysis, properties, applications in C-C coupling reactions (Suzuki-Miyaura, Heck, Sonogashira), alcohol oxidation reactions, epoxidation reaction, transfer hydrogenation reaction, carbonylation of methanol to acetic acid, hydrogenation of olefins, mechanisms. 20

(ii) Introduction, immobilization of metal complexes in various supports like Silica, Alumina, Zeolite, etc. Supported metal Nanoparticles. Characterizations of supported materials by XRD, SEM, TEM, XPS, BET, etc. Applications of supported catalysts. 10

Books / Reference recommended

(i) Physical methods of Chemists: R. S. Drago
(ii) The Organometallic Chemistry of the Transition Metals, 5th Edition, by Robert H. Crabtree.
(iii) Steric effects of phosphine ligands in organometallic chemistry and catalysis, C. A. Tolman, Chem. Rev. 1977, 313.
(iv) Inorganic Chemistry Principles and Structure –J. E. Huheey

Ph.D. Course Work
Course: III
A Fundamental Approach to Inorganic Synthesis and Analysis (Optional)
Course Teacher : Prof. G. Borah
Marks 60 + 40 (Int. Ass) = 100

Unit I: Different types of ligands (e.g. Schiff-Base, Hemilabile, Pincer types etc.) Synthesis and their properties. **Marks:10**

Unit II: Modern methods applied in Inorganic and Organometallic synthesis. Handling of air and moisture sensitive compounds, drybox, glove bag, Schlenk line and vacuum line techniques. Methods of purification and crystallization of solids for x-ray analysis. General strategies, brief outline of theory and methodology used for synthesis of transition metal complexes, a few examples of detailed specific synthesis of some complexes with justification of the methodology adopted . Application of transition metal complexes in catalysis (e.g. Cross-Coupling reactions, Oxidation reactions, etc.)

Marks:25

Unit III: Application of Electronic spectroscopy in characterization of inorganic complexes, multinuclear NMR (^{31}P, ^{15}N, ^{19}F) spectra of inorganic complexes, EPR spectra of Vanadium, Copper, Cobalt and Iron complexes. Mass spectroscopic methods used in inorganic chemistry, determination of magnetic properties, application of electro analytical tools (e.g. Cyclic voltammetry, polarography) in characterization of transition metal based compounds.

Marks:25

Books recommended:

1. Organometallic chemistry of Transition Metals: R.H. Crabtree, John Wiley & Sons, 2001.
2. Structural Methods in Inorganic Chemistry: E.A.V. Ebsworth, David W.H. Rankin , Stephen Cradock (2nd edn) , Blackwell scientific Publications
3. Electronic Spectra of Transition Metal Complexes: D.Sutton , (McGraw-Hill, London) 1968.
4. Electronic Spectroscopy : A.B.P. Lever
5. Instrumental Methods of Chemical Analysis: Gurdeep R. Chatwal & Sham K. Anand.

Ph.D. Course Work
Course-III
Advances in Metal Carbene Chemistry (Optional)
Course Teacher: Dr. Ramananda Maity
Marks 60 + 40 (Int. Ass) = 100

Unit I: Synthesis and reactivity of carbenes **Mark 30**

Different types of carbenes, electronic structure and stability of carbenes, influence of substituent on stability, MO diagrams, N-heterocyclic carbenes (NHCs), synthesis of free NHCs, reactivity of stable singlet carbenes, 1,2-migration reactions, carbene dimerization and related reactions, carbene-carbenoid coupling reactions, insertion reactions, carbene-lewis acid adducts, carbene-lewis base adducts, carbene precursors and their synthesis, synthesis of transition-metal carbene complexes, phosphinocarbene complexes, catalytic applications of free carbenes, asymmetric catalysis using chiral carbenes.

Unit II: Characterization and applications of carbene complexes **Marks 20**

Characterization of carbene complexes by ^{1}H, $^{13}C\{^{1}H\}$, 2D correlation spectroscopy, mass spectrometry and X-ray crystallography, applications of carbene complexes in various organic transformations such as Heck-type reactions, hydrogenation of olefins, hydrosilylation reactions and polymerization of alkynes, Polynuclear carbene complexes for cooperative catalysis, cyclometalated carbene complexes and their applications in catalysis.

Unit III: Supramolecular complexes using carbene ligands **Mark 10**

Supramolecular interactions, supramolecular structures with N-donor ligands, supramolecular architectures using carbene donor ligands and their importance.

References:

(a) Hahn, F. E.; Jahnke, M. C. *Angew. Chem., Int. Ed*. **2008**, *47*, 3122−3172. (b) Bourissou, D.; Guerret, O.; Gabbaı, F. P.; Bertrand, G. *Chem. Rev.* **2000,** *100,* 39-91. (c) Albrecht, M. *Chem. Rev.* **2010,** *110,* 576–623. (d) Weskamp, T.; Böhm, V. P.W.; Herrmann, W. A. *J. Organomet. Chem.* **2000**, *600*, 12–22.

Ph.D. Course work
Paper III
Organic Synthesis (Optional)
Course Teacher : Prof. J.G. Handique
Marks 60 + 40 (Int. Ass) = 100

Unit 1: Retrosynthetic analysis in Organic synthesis Marks 35

Review on the basics of retrosynthetic analysis, Criteria for good disconnection, Concepts of acceptor and donor synthons, Use of reversal of polarity (Umpolung).

One group disconnection: Disconnection and synthesis of alcohols, olefins, simple ketones, acidsand its derivatives.

Two group Disconnection: Disconnection in 1,3-dioxygenated skeletons, preparation of β-hydroxy carbonyl compounds, α, β-unsaturated carbonyl compounds, 1,3- and 1,5-dicarbonyl compounds. Use of Mannich Reaction,Michael Addition and Robinson annulation, control of carbonyl condensation.

Illogical two group disconnections: Disconnection and synthesis of 2-hydroxy carbonyl compounds, 1,2-diols, 1,4 and 1,6-dicarbonyl compounds.

Other difunctionalised compounds: 1,2-, 1,3-, 1,4-, 1,5- and 1,6- difunctionalised compounds.

Unit 2: Reactions of synthetic importance Marks 25

Study of following reactions, their mechanism and synthetic utility: Mitsunobu reaction, Baylis-Hilman reaction, Sharpless asymmetric epoxidation, dihdroxylation and aminhydroxylation, Wohl-Ziegler bromination, Wittig-Horner Reaction, Henry reaction, Peterson olefination, Pd-catalyzed coupling reactions.

Books Recommended:

1. Organic Synthesis: The Disconnection Approach By S. Warren, Wiley
2. Designing Organic Synthesis : A Programmed Introduction to the Synthon approach - By S. Warren, Wiley
3. Organic Chemistry – Paula YurkanisBruice, Pearson
4. Organic Chemistry- Clayden, Greeves, Warren and Wothers, Oxford University Press.
5. Advanced Organic Chemistry Part A and B : Carey and Sundberg
6. Modern Methods of Organic Synthesis – Carruthers and Mendham, Cambridge University Press
7. Organic Synthesis – M.B. Smith, McGraw Hill. (Reference book)
8. Principles of Organic Synthesis – R.O.C. Norman and J M Coxon
9. Advanced Organic Chemistry: Reactions, Mechanisms and Structure By J. March, Wiley
10. Organic Synthesis - Concepts, Methods and Starting Materials By J. Fuhrhop and G. Penzilin, Verlag VCH

Ph.D. Course Work
Course-III
Green Chemistry and Environment (Optional)
Course Teacher: Dr. D. Sarma
Marks 60 + 40 (Int. Ass) = 100

Unit-I: Green Chemistry **Marks-30**

Principles of green chemistry; Concept of Atom Economy; Green starting materials, Green reagents, Green solvents (Water, Ionic liquid, Polyethylene glycol, Super Critical Fluids, etc), Green reactions, Green products, Green Catalysts.

Solid supported organic reactions: Catalysis by solid acids and bases; Use of clay in green synthesis; PTC catalyzed green reactions; Biocatalysis; Sonication and Microwave assisted organic synthesis; DMC, TBAB and Rongalaite as green reagents in organic synthesis

Green synthesis of Acetanilide, Ibuprofen, Adipic acid, Urethane, Catechol, BHT (Butylated Hydroxy Toluene).

Unit-II: Environmental Chemistry: Environmental Pollution from Agriculture-Pesticides **Marks-30**

Definition, Importance and general classification of agrochemicals, classification of pesticides on the basis of chemical nature, mode of action and target species.

An introduction to structure, chemical nature, physical properties, chemical properties, synthesis, degradation metabolism formulations, uses, toxicities (Acute, dermal and chronic toxicities in mammals, birds, aquatic species etc.) etc. Methods of pesticide analysis.

Recent advances in pest control: green chemistry in pesticides; Botanical and bio pesticides.

Books recommended:

1. Principles of Green Chemistry : Paul Anastas and J Werner
2. Green Chemistry : V.K. Ahluwalia
3. Robert, D.A. 1978. Fundamentals of Plant Pest Control. Freeman and Co. USA.
4. Chemistry of Insecticides and fungicides-U.S. Shree Ramulu Oxford and IBH Pub., 2nd 1995
5. Pesticide Synthesis by P.S.Marg, G.K.Kohn, J.J.Menn
6. Analytical methods for pesticides, plant growth regulator and food additives. Vol, I-IV Ed by Gunter Zweig.
7. Pesticide formulations recent development and their application in developing countries by Wade van Valkenburg, B. Sugavanam, Sushil K. Khetan, UNIDO, 1998.
8. Chemistry of pesticides by K. H. Buchel
9. Analysis of Pesticide residues by H. A. Moye
10. Environmental Chemistry by A. K. Dey

Ph.D. Course work
Course III
Supramolecular, Natural Products and Medicinal Chemistry Chemistry (Optional)
Couse Teacher: Dr. B. Chetia
Marks 60 + 40 (Int. Ass) = 100

Unit I: Supramolecular Chemistry Marks 30

Definition, Concepts of host guest complexation, classification, thermodynamics and kinetic stability, Non-covalent interactions, Supramolecular design, Molecular recognition, Recognition of anionic substrates, Cation binding, Supramolecular reactivity and catalysis, Effects of medium, Chiral recognition, Biological self-assembly.

Molecular receptors for different types of molecules: Crown ethers, cryptands, cyclodextrins, Calixarenes.

Molecular devices: ionic, electronic and switching devices.

Books Recommended:

1. Supramolecular Chemistry, J.M. Lehn, VCH, New York, 1995
2. Supramolecular Chemistry, J. W. Steed and J. L. Atwood; John Wiley & Sons, Ltd
3. H.J. Schneider and A. Yatsimirsky, Principles and Methods in Supramolecular Chemistry.

Unit II: Natural Products and Medicinal Chemistry Marks 30

Definition of drugs and factors affecting their bioactivity, Definition of chemotherapeutic index and therapeutic index, Discovery of new drugs: drug discovery without a lead (penicillins, Librium), Lead discovery, random screen, nonrandom (or targeted or focused) screening, drug metabolism studies, rational approaches to lead discovery, Lead modification (drug design and development), functional group modification, structure-activity relationship, clinical trials (phase-0, Phase-I, Phase-II, Phase-III, Phase-IV clinical trials).

Prostaglandins: Occurrence, classification, biogenesis and physiological effects, synthesis.

Total synthesis of following complex natural products (discuss stepwise chemistry, stereochemistry, reagents used etc.): Morphine, Tolterodine, Nakiterpiosin, Varitriol, taxol

Books Recommended:

1. The Organic Chemistry of Drug Design and Drug Action (2nd Ed), R. B. Silverman, Academic Press
2. Medicinal Chemistry – A. Kar, Wiley Eastern Ltd., New Age International Ltd., New Delhi
3. Medicinal Chemistry – A. Burger (ed). Interscience, New York

References:

2. Total Synthesis of Tolteridine (Ref *J. Org. Chem*. **2009**, 74, 4232)
3. Total Synthesis of Nikiterpisonin (Ref *J. Am. Chem. Soc*. **2009**, 1410)
4. Total Synthesis of Varitriol (Ref J. Org. Chem. 2013, 78, 8840-8846)
5. Total synthesis of prostaglandins E_2 and $F_{2\alpha}$ (*Tetrahedron Letters*, **1970**, 307)

Ph.D. Course work
Course III
Computational Chemistry (Optional)
Course Teacher : Dr. R. Kar
Marks 60 + 40 (Int. Ass) = 100

Introduction to Computational Chemistry: Representation of molecules, Geometry Optimization, Frequency calculation, Calculating thermodynamic functions, Born-Oppenheimer Approximation, potential energy surface.

Basis sets: Gaussian basis functions, correlation consistent basis sets, basis-set superposition error. Introduction to electronic structure software (Gaussian, GAMESS).

Review of the Hartree-Fock approximation. Fock operator and canonical representation, restricted closed-shell Hartree-Fock theory, Interpretation to Hartree-Fock solutions, Illustration of closed-shell calculation.

Basic Principles of density functional theory, non-interacting model of Kohn-Sham, Exchange-Correlation Functionals, General Performance and Applications of DFT. Density-based reactivity theory: Concepts and application of global and local reactivity descriptors. Basic idea and applications of time-dependent density functional theory

Introduction to FORTRAN: Constants, variables and expressions, input and output statements, format specifications, control statements, nesting of loops, arrays and subscripted variables, functions and subroutines.

Data fitting by least square, Newton–Raphson and iterative methods for solving non-linear equations; Linear simultaneous equations - Cramer's rule, Gauss elimination method and Gauss-Seidel method; Numerical integration, interpolation, Gauss's quadrature formula; trapezoidal method, Simpson's 1/3 rule.

Recommended Books:

1. Introduction to Computational Chemistry, Frank Jensen, Wiley
2. Modern Quantum Theory – N. S. Ostlund and A. Szabo, McGraw Hill.
3. Density functional theory of atoms and molecules, R.G. Parr and W. Yang, Oxford.
4. Methods of Molecular Quantum mechanics, R. McWeeney and B. T. Sutcliffe, Academic Press.
5. FORTRAN & Numerical Methods, C. Xavier, New Age International Publishers

PhD Course work

Paper- III

Carbon based Polymer nanocomposites

Course Teacher: Dr. Surajit Konwer

Credit: 4 **Total Marks 100 (End Semester 60: Internal Assessment 40)**

Unit I: Nanomaterials

Definition, Types of nanostructures, Properties and Applications: One dimensional, Two dimensional and Three dimensional nanostructured materials, Quantum Dots shell structures, metal oxides, semiconductors, composites, mechanical-physical-chemical properties, polymer based application, basic principle. Synthesis and preparation of Nanomaterials and Synthetic Techniques: Synthesis of bulk nanostructured materials - Sol Gel processing- bulk and nano composite materials and electrochemical approaches.

Marks 10

Carbon nanostructures: Synthesis, separation and characterization of Fullerene and its derivatives, applications, toxicity. Carbon nanotube (CNT), structure, synthesis and functionalization of CNT, electronic, vibrational, mechanical and optical properties of CNT, applications. Graphene, structure, synthesis and functionalization of Graphene, Graphene composites, electronic applications of Graphene, Graphene Oxide.

Marks 15

Unit II: Advanced electrochemistry: Electrolyte to polyelectrolytes

The extension of Debye-Hückel limiting law; Pitzer ion-interaction approach for osmotic and activity coefficients of electrolyte solutions; Debye-Hückel-Onsager theory for electrical conduction in electrolyte solutions; limitation of Debye-Hückel-Onsager theory.

Poisson-Boltzmann cell model of polyelectrolyte solutions; osmotic and activity coefficients of polyelectrolytes; vapor pressure osmometry; electrical conductivity of polyelectrolyte solutions.

Principle and application of Cyclic Voltammetry (CV), Randles Sevick equation, electrode used in CV. Impedance Spectroscopy.

Marks 20

Unit III: Conjugated Polymers

Basic concepts of terms used in Polymers, Importance, Classification of Polymer, Polymerization condition & techniques. Conjugated polymer: synthesis and applications, conduction mechanism of conducting polymers, metallic character and nanostructure of conducting polymers. Fillers, theory of effect of fillers reinforcements, coupling agents, composites, nanocomposites, Intercalative & exfoliate.

Marks 15

Reference Book:

1. Handbook of Conducting polymers: Processing and Application edited by Terje A. Skotheim and Jhon R. Reynolds
2. Modern Electrochemistry – Vol I, II by J. O. M. Bockris & A. K. N. Reddy

PhD Course Work
Paper-III
Introduction to Protein Biophysics
Course Teacher: Dr. Anupaul Baruah

Credit 4 Total Marks 100 (End semester 60: Internal Assessment 40)

Unit I: Protein folding Marks 15

Structure of proteins, Levinthal Paradox, Concept of energy landscape, different models of protein folding kinetics and thermodynamics

Unit II: Marks 25

Protein misfolding: Protein homeostasis, theories of protein misfolding, Misfolding diseases

Protein Disorder: Sequence-structure-function paradigm, sequence properties of intrinsically disordered proteins

Protein Design: models and methods of protein design, advances in protein design.

Unit III: Marks 20

Statistical Mechanics: Concept of ensemble, time average, ensemble average, Postulates.

Methods: Basics of Monte Carlo simulation and Molecular Dynamics simulation and its application to protein biophysics, Mean field theory and its application,genetic algorithm and its application, neural network and its application, Docking and its application.

Ph.D Course Work
Course-III
Green Energy Materials and its Processing
Course Teacher: Dr. G. Sharma (DUIET)
Full Mark 100 (Internal assessments: 40; End Semester: 60)

Unit 1: Introductionto green energy materials; Sustainable energy: Organic solar cells, Dye-sensitized solar cells (DSSCs), polymer solar cells, hybrid polymer solar cells, polymer based light emitting diodes. Newer Energy Materials: Carbon nano-tubes (CNTs) and multiwall carbon nanotubes (MWCNTs) -methods of production, properties and its utility in energy devices. Polymers and composites -classification, methods of production, properties, fabrication methods, and its utility in making energy devices. Recent advances in new energy materials. Marks-30

Unit 2: Silicon processing methods: Dry and wet chemical processes used to develop new materials and micro-engineered products. Principles for photovoltaic and their relevance in current energy industry. Fabrications: Gas-solid and liquid-solid reactions-their role in micro engineering. Various reactors and methods of fabrication methods, such as physical and chemical vapour deposition techniques, photolithography, electroless and electrochemical deposition, etching, and through mask plating and common models to describe these processes. Marks-30

References

1. R Kirkwood and A Longley, Clean Technology and the Environment, Blackie October 1994.
2. A. Johansson, Clean Technology", Lewis 1992.
3. M. Charter and U. Tischner, Sustainable Solutions, Greenleaf Publishing, 2001.
4. V. R. Gowarikar, N.S. Viswanathan, J. Sreedhar, Polymer science, sixth reprint 1993.
5. G.S. Misra, Introductory Polymer Chemistry, 1993
6. F.L. Mathews F.L. Chapman and Hall, Composite materials: Engineering and science, 1994
7. Frederick C. Krebs, Polymer photovoltaics- A practical approach, SPIE Press, 2008.
8. M. Graziani and P. Fornasiero, Renewable resources and renewable energy- A global challenge, CRC-Taylor and Francis, 2007.

Syllabus for Ph.D.
Course III
Instructor: **Jiban Saikia**

Course Title: Biomaterials for Sustainable Agriculture

Credit 4 **Total Marks 100 (End semester 60: Internal Assessment 40)**

Unit I Mark 20

Bio-fertilizer: Introduction to Bio-fertilizers, their types and their functions. Advantages and disadvantages of bio-fertilizers over chemical fertilizers. Encapsulation and release of bio-fertilizers from different matrix. Isolation, characterization and culturing techniques of different bio-agents for bio-fertilizer. Production of bio-fertilizer microbes,Commercial bio-formulation and its production techniques.

Unit II Mark 20

Nanotechnology in Agriculture. Natural nanoparticles and their role in soil and water quality: Use of Nanotechnology for the mitigating theimpacts of Drought and arresting DesertificationWater retaining soil conditioners. Super absorbent polymers (SAPs). Synthesis andCharacterization - Zeolites –Nano emulsion based antitranspirants.Nano particles and mesoporous nanomaterials for smart delivery of pesticides/herbicides/bio-fertilizers.

Unit III Mark 20

Foliar Delivery of Nutrients to Plants: Delivery of agro-materials through plant cuticle membranes. Definition of foliar fertilization. Absorption of foliar-applied nutrients. Structure and function of the leaf cuticle. Factors affecting foliar fertilization. Sorption interactions of plant cuticular matter with organic/inorganic compounds. Advantages and disadvantages of foliar fertilization.

Pheromones for pest management. Pheromone encapsulation/entrapment for increasing the effectiveness and shelf-life.

PhD Course work
Course: Nanostructured Materials (PhD)

Instructor: **Kalyanjyoti Deori**

Credit 4 Total Marks 100 (End Semester 60 + Internal Assessment 40)

Unit I: Introduction to Nanoscience and Nanotechnology Marks: 30

Background to Nanoscience, size effects and crystals, large surface to volume ratio, surface effects on the properties. Types of nanostructure and properties of nanomaterials: One dimensional, Two dimensional and Three dimensional nanostructured materials, Quantum Dots shell structures, metal oxides, semiconductors, composites, mechanical-physical-chemical properties. Quantum confinement effect and Surface plasmon resonance. Introduction to surface active agents: theory and applications, types of surfactants. Origin of colloidal particles, preparation & characterization of colloidal particles.

Unit II: Synthesis and applications of nanostructured materials Marks: 30

Synthesis and modification of nanoparticles**:** Top-Down and Bottom-Up approach, experimental procedure (coprecipitation, Sol-gel, Hydrothermal, colloidal etc.), Properties of precipitates and precipitating reagents: Colloidal and Crystalline Precipitates, nucleation (homogeneous and heterogeneous), crystal growth, crystallography and morphology dependence properties. Basic characterizations for structural purity and morphology study. Applications of nanoparticles in catalysis (photocatalysis, electrocatalysis etc.), energy, biology and medicine, and in everyday life.

Course III
Supramolecular chemistry and its applications
Subject instructor: Dr. Prithiviraj Khakhlary

Credit: 4 Marks: (Semester 60+ Internal Assessment 40)

Unit I
Hydrogen Bonding: Definitions, Hydrogen bond Donors and Acceptors, Strong Vs Weak Hydrogen Bonds, Abundant Vs Rare Hydrogen Bonds, Analysis of Hydrogen Bonding.
Marks 20

Unit II
Molecular Recognition and Self-Assembly: Introduction and applications
Polymorphism, Crystal Transformations: Introduction and applications
Marks 20

Unit III
The One-, Two- and Three-Dimensional Organic-Inorganic Hybrid Materials: Introduction and Solid-Gas Interactions between Small Gaseous Molecules and Transition Metals in the Solid State.
Marks 20

Reference books:

1. Crystal Design: Structure and Function by G. R. Desiraju
2. Supramolecular Chemistry by Jonathan W. Steed

Ph.D. Course Work

Course IV (Assignment)

Total : 100

[Marks 80 (assignment writing) + 20 (viva on the assignment)]

Students have to complete the assignment work (practical/review) under guidance of the prospective Supervisor concerned.