Consolidation of all changes brought about in the of Ph. D Course work Syllabus (Proposed to be effective from 2017 Session)

1. Paper-II: Essentials in Chemical Science Research

New syllabus has been prepared for this paper. The paper consists of Four units, having 4 credit points (100 marks). The Topics incorporated in this paper are:

UNIT-I: Mathematical Chemistry UNIT-II: Application of Computer in Chemical Science Research UNIT-III: Instrumental Techniques UNIT-IV: Safety Measures and Waste Management in Chemical Laboratory

2. The one paper for **Paper-III** has been **replaced** with **three optional papers** as follows:

Paper-III(A): Materials Chemistry Paper-III(B): Advanced Organic Chemistry Paper-III(C): Topics in Advanced Chemistry

(The candidate has to choose any one from these three optional papers) New syllabus has been prepared for each of these papers

DEPARTMENT OF CHEMISTRY ASSAMUNIVERSITY: SILCHAR

Syllabus for IPP Course Work to be effective from 2017 Session

Course Structure

| Course Number | Course Name | Nature | Max Credit | Max Marks |
|------------------|---|------------------|---------------|--------------|
| Paper-I | Research Methodology | School Level | 4 | 100 |
| Paper-II | Essentials in Chemical Science Research | Department Level | 4 | 100 |
| Paper-III(A) | Materials Chemistry | Department Level | 4 | 100 |
| Paper-III(B) | Advanced Organic Chemistry | Department Level | 4 | 100 |
| Paper-III(C) | Topics in Advanced Chemistry | Department Level | 4 | 100 |
| Paper-IV | Term Paper | | 4 | 100 |
| Total | | 16 | 16 | 400 |



ALBERT EINSTEIN SCHOOL OF PHYSICAL SCIENCES ASSAM UNIVERSITY, SILCHAR COURSE WORK SYLLABUS FOR Ph. D/M. Phil

Paper – 1: Research Methodology in Physical Sciences (School Level)

Credit: 04

UNIT –I:

Research: Meaning, objectives, types, approaches. Criteria of good research, research problems, research design. Review of literature: Meaning, objectives, principles and procedure. Report writing: Meaning, significance, types, techniques.

UNIT – II:

Quantitative methods of research: Methods of data collection – experimental data, field data, data from secondary sources. Relation between variables: correlation (both continuous & binary data), regression (both linear & non-linear) for two variables. Test of significance including one-way-anova. Errors and analysis of errors.

UNIT – III:

Computer application in research: Data analysis – use of software like Excel/Mat lab/Mathemetica/SPSS etc., Word processing – use of software like MS Word/LATEX/End Note etc., Data bases – use of software like MS Access/My SQL etc. Introduction to Computer Network: Network Protocol and topology. Computer simulations: Introduction to mathematical and simulation models, deterministic and stochastic simulation models, continuous and discrete simulation.

UNIT – IV:

Intellectual Property Rights (IPR) – patents, copyrights and related issues. Plagiarism: concept, software, legal aspects. National Science Policies, Ethics in Research

Suggested readings:

- 1. Research Methodology-Methods and Techniques, New Age International, C. R. Kothari, 2nd Ed. (New Delhi), 2008.
- 2. Research Methodology: A step-by-step guide for beginners, SAGE Publications, Ranjit Kumar, 2005.
- 3. Mastering MATLAB by Duane C. Hanselman and Bruce L. Littlefield, 2011.
- 4. Queqeing system-Vol.2-D, Kleinrock, John Wiley & Sons Inc New York, 1976.
- 5. Computer Network by A. Tanebaum. Printice Hall Ind. Englewood cliffs N.J., 1981.
- 6. Data and computer communications by W. Stallings, Mc Millan Pub. Co. New York, 1976.

Paper-II Essentials in Chemical Science Research Max. Marks: 100 Credit: 4

UNIT-I: Mathematical Chemistry

Mathematical Foundations, Characterizing Measurements and Results, Characterizing Experimental Errors, Statistical Analysis of Data, Statistical Methods for Normal Distributions, Standardizing Methods, Linear Regression and Calibration Curves

UNIT-II: Computer in Chemical Science Research

A brief outline of molecular mechanics, semi-empirical approximations, *ab initio* methods, Density functional theory methods, basis set types and sizes and Z-matrix; Potential energy surface, local and global minima, Molecular Force-field calculations. Development of small computer codes (in FORTRAN or C) to solve chemical problems.

UNIT-III: Instrumental Techniques

Basic concepts & application related to the following instrumental techniques: FT-IR spectroscopy, Raman spectroscopy, Spectrofluorimetry, GC-MS, Powder XRD Microscopic Techniques: Polarised Optical microscopy, AFM, SEM, TEM, STM, EDX. FT-NMR: Rules for spectral analysis, 2-D NMR & application of COSY, NOESY, ROESY

UNIT-IV: Safety Measures and Waste Management in Chemical Laboratory

Safety measures: Protective gears, laboratory emergencies, Case studies of incidents and Lesson learned, Managing and Working with Chemicals: Chemical Segregation, Transfer and Transport, Chemical Fume Hood, chemical hazards, Use of MSDS, Waste handling: Characterization of Waste, Collection and Storage, Solid Wastes.

Suggested Readings:

- 1. Franck Jensen, Introduction to computational chemistry, 2nd Ed., John Wiley & Sons Ltd. (2007).
- 2. Drago, Principles of Instrumental Techniques" H.H.Willard, L.L. Merritt.Jr and J.A.Dean, Instrumental Methods of Analysis, Van Nostrand Company, New York (1965) Revised edition-2008.
- 3. TensiometryHeideSchatten and J.B.Pawley, Biological "Low Voltage Scanning Electron Microscope" Springer (2007) ,ISBN-10:0387729704.
- 4. D.C.Bell, Energy Dispersur X –Ray Analysis in the Electron Microscope ,BIOS Scientific Publisher Ltd.(2003).

Paper-III (A) Materials Chemistry Max. Marks: 100 Credit: 4

UNIT-I: Liquid Crystals

Plastic Crystals and Liquid Crystals, Classification, General synthetic strategies of thermotropic liquid crystals, Order parameters for cholesteric, nematic and smectic phase and their experimental determination, Optical properties and defects in liquid crystals, Diffraction of X-rays by liquid crystals, Information obtained from X-ray studies on liquid crystalline materials. Electrical and Magnetic properties of liquid crystals, Theory of dielectric anisotropy, Freedericksz effect, application of liquid crystals.

UNIT-II: Metallomesogens

Definition, examples, strategies for synthesis of metallomesogens, functionalisation of multidentate ligands (salen, salphen type etc.). Metallomesogens involving copper, vanadium, nickel, palladium, platinum, lanthanides etc. Study of their properties, like NLO, photoluminescence etc.

UNIT-III: Properties and Applications of Nanoscale Materials

Nanoscale Materials: Definition – Size effect Synthesis – Some Typical Chemical approaches Properties – Optical, Electronic, Catalytic and Magnetic, Applications in Solar Cell, Catalysis, and Photodynamic Therapy.

UNIT-IV: Carbon Nanomaterials

Carbon Nanotubes: Definition, Different Types-Single and Multi-Walled, Synthesis-Some Typical Examples, Properties and Applications. Environmental Impacts and Health Hazards

Suggested Readings

- 1. Introduction to Nanoscale Science and Technology, (Ed) M.D.VentraS.Evoy and J.R.Heflen Kluwer Academic Publisher, Boston., (2004).
- 2. Nanometerials Chemistry: Resent Developments and New Directions" C.N.R. Rao, A.Muller and A.K.Cheetham, Wiley VCH (2007).
- **3.** Chemistry of Nanomaterials", C.N.R Rao, A.Muller and A.K.Cheetham (Eds) Wiley-VCH, Weinheim, 2004, Reprinted 2006.
- 4. Liquid Crystals: Fundamentals, David A. Dunmur and Shri Singh, World Scientific Publishing Co Pte Ltd, 2000
- 5. Nanoscience with Liquid Crystals, Quan Li (Editor)Springer; 2014 edition

Paper-III (B) Advanced Organic Chemistry Max. Marks: 100 Credit: 4

UNIT-I: Application of Computer in Chemical Science Research

Application of computational methods for prediction of chemical Potential, Electronegativity, Hardness and Softness of molecules. DFT Formulation of Reactivity—The Fukui Function. Electronic structure and thermochemical properties, geometry optimization, study of reaction mechanism, transition-state optimizations.

UNIT-II: Carbohydrates

Carbohydrates: Structure of Monosaccharide. Importance of carbohydrates (Carbohydrates as antibiotics, Vaccines, Tumor metastasis etc.) Structural features of Polysaccharides, Glycoprotein, Proteoglycans.

Synthesis : Glycosyl Donor, Glycosyl Acceptor, Techniques of oligosaccharides synthesis. Synthesis and Applications of Carbohydrate-Derived Macrocyclic Compounds

UNIT-III: Organic Photosensitizers

Biomedical Organic Photosensitizers: Porphyrin analogues, nucleic acid analogues, functionalization of carbon nanomaterials with organic molecules in the development of photosensitizers. Photodynamic therapy and applications, Photo thermal therapy, Hyperthermia

UNIT-IV: Organic Reaction Methodology

Designing organic synthesis, Multi-component reactions for the synthesis of heterocyclic and biologically active molecules, Ugi Reaction, Passerini Reaction, Organocatalysis.

Suggested Readings

- 1. Organic Synthesis with Carbohydrates, Geert-Jan Boons, Continuum International Publishing Group - Sheffie
- 2. Carbohydrate Chemistry, Geert-Jan Boons, Springer
- 3. Computational Chemistry, D Jolly, Ivy Publishing House
- 4. Computational Chemistry : Intro To The Theory & Applications Of Molecular & Quantum Mechanics, Errol Lewars, Springer
- 5. Computational Chemistry (Oxford Chemistry Primers), Guy H. Grant, OUP Oxford
- 6. Computational Chemistry: A Practical Guide for Applying Techniques to Real World Problems, David Young, Wiley-Blackwell
- 7. Photosensitizers in Medicine, Environment, and Security, T. Nyokong (Editor), Vefa Ahsen (Editor), Springer
- 8. Towards Dual and Targeted Cancer Therapy with Novel Phthalocyanine-based Photosensitizers, Janet T F Lau, Springer
- 9. Designing Organic Synthesis, Sharma, Pragati Prakashan
- 10. Designing Organic Syntheses: A Programmed Introduction to the Synthon Approach, Stuart Warren, Wiley-Blackwell
- 11. Multicomponent Reactions: Concepts and Applications for Design and Synthesis, Raquel P. Herrera, Eugenia Marqués, Wiley-VCH, Weinheim, 2015

Paper-III (C) Topics in Advanced Chemistry Max. Marks: 100 Credit: 4

UNIT-I: Application of Transition Metal Complexes

Binding of transition metal complexes with DNA and Nucleic Acid, Anticancer activity of Platinum Group Complexes: different type of active complexes, Antimicrobial activity of metal chelates.

Alkaline phosphatase: structure and reactivity; Insulin: structure and reactivity.

UNIT-II: Catalysis

General Principles, Energetics, Catalytic cycles, Catalytic efficiency and lifetime, Selectivity, Homogeneous catalysis: Alkene metathesis, Asymmetric oxidation, Palladiumcatalyzed C-C bond forming reactions, Methanol carbonylation, Heterogeneous catalysis: Surface area and porosity, Surface acidic and basic sites, Surface metal sites, Chemisorption and desorption, Hydrogenation catalysts, Sulfur dioxide oxidation, Electrocatalysis, Hybrid catalysis: Tethered catalysts, Biphasic systems

UNIT-III: Application of Fluorescence

Types of Photophysical Pathways, Fluorophores, Quenching of Fluorescence, Energy Transfer and Protein Fluorescence.

UNIT-IV: Chemical and Electrochemical Kinetics and Environment Related Chemistry

Electrochemistry Fuel cells; Solar cells (photochemical, photovoltaic); Batteries (solid-state & conventional)-single electrode and complete cell studies; Production of H₂ and important chemicals of high energy; Corrosion & waste removal techniques

Suggested Readings

- 1. Shriver& Atkins' Inorganic Chemistry, P. Atkins, T. Overton, J. Rourke, M. Weller, F. Armstrong, Fifth Edition, Oxford University Press.
- 2. Protein Fluorescence, Joseph R. Lacowicz, Springer
- 3. Single-Molecule Fluorescence Spectroscopy of the Folding of a Repeat Protein, Sharona Cohen, Springer

Paper-IV Term Paper Max. Marks: 100 Credit: 4

A prospective Ph. D scholar shall prepare a term paper (not exceeding 10-15 pages) which will involve both a report as well as a presentation on the subject area of his/her Ph. D topic including objectives / literature review, etc. This term paper shall be guided by the supervisor.