SYLLABUS OF COURSE WORK

OF

DOCTOR OF PHILOSOPHY

(w.e.f. Academic Session: 2020-2021)

Department of Chemistry

(Faculty of Science & Technology)

Aliah University

IIA/27, Newtown, Kolkata 700160, West Bengal, India

Contents

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PHD/RM-01	Research Methodology	04
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2. Detailed Syllabi

Course name: Research Methodology
Course code: PHD/RM-01; Credit: 4
Lecture: 40

Identification of the Problem: Identifying and design/formulating the problem.

Solving the problem:
a) Analytical methods
b) Numerically solving
c) Simulation by computer programming
d) Experimental observations
e) Theoretical modeling

Developing a research plan: Objective; Steps for solving the problem; Description of approach, Stating any assumptions; Details of techniques

Data collection: Experimental data, field data, theoretically obtained data

Analyzing data: Error analysis, statistical analysis

Computational approach:
1. Literature survey: Using web, handling search engines
2. Computer usage: For collecting/analyzing data; simulations; graphical and pictorial representation.
3. Preparing presentations:
i) Research papers: Using word processing software – MS Word/Latex/others, Drawing graphs and diagrams – Origin/Excel/ChemDraw/Photoshop/Others.
ii) Seminar presentations – Power point for oral and poster presentations

Course name: Research and Publication Ethics
Course code: PHD/RPE-02; Credit: 2
Lecture: 20

PHILOSOPHY AND ETHICS (3 hrs.)

1. Introduction to philosophy: definition, nature and scope, concept, branches
2. Ethics: definition, moral philosophy, nature of moral judgements and reactions

SCIENTIFIC CONDUCT (5hrs.)

1. Ethics with respect to science and research
2. Intellectual honesty and research integrity
3. Scientific misconducts: Falsification, Fabrication, and Plagiarism (FFP)
4. Redundant publications: duplicate and overlapping publications, salami slicing
5. Selective reporting and misrepresentation of data

PUBLICATION ETHICS (7 hrs.)

1. Publication ethics: definition, introduction and importance
2. Best practices / standards setting initiatives and guidelines: COPE, WAME, etc.
3. Conflicts of interest
4. Publication misconduct: definition, concept, problems that lead to unethical behavior and vice versa, types
5. Violation of publication ethics, authorship and contributorship
6. Identification of publication misconduct, complaints and appeals
7. Predatory publishers and journals

OPEN ACCESS PUBLISHING(4 hrs.)

1. Open access publications and initiatives
2. SHERPA/RoMEO online resource to check publisher copyright & self-archiving policies
3. Software tool to identify predatory publications developed by SPPU
4. Journal finder / journal suggestion tools viz. JANE, Elsevier Journal Finder, Springer Journal Suggester, etc.

PUBLICATION MISCONDUCT (4hrs.)

A. Group Discussions (2 hrs.)
   1. Subject specific ethical issues, FFP, authorship
   2. Conflicts of interest
   3. Complaints and appeals: examples and fraud from India and abroad

B. Software tools (2 hrs.)

Use of plagiarism software like Tumitin, Urkund and other open source software tools

DATABASES AND RESEARCH METRICS (7hrs.)

A. Databases (4 hrs.)
1. Indexing databases
2. Citation databases: Web of Science, Scopus, etc.

B. Research Metrics (3 hrs.)
1. Impact Factor of journal as per Journal Citation Report, SNIP, SJR, IPP, Cite Score
2. Metrics: h-index, g index, i10 index, altmetrics

Course name: Literature Review, Report and Seminar Presentation
Course code: PHD/LR-03; Credit: 4
Lecture: 40

The relevance of the research project from perspective of the subject.
Detailed review of state of the art.
Scope of the work.
Significance of the project.
Expected outcome.

Course name: Subject Paper (Supramolecular Chemistry)
Course code: PHD/SP-04; Credit: 4
Lecture: 40

Definition of supramolecular chemistry

Nature of binding interactions in supramolecular structures: ion-ion, ion-dipole, dipole-dipole, H-bonding, cation-p, anion-p, p-p, and van der Waals interactions.
Synthesis and structure of crown ethers, lariat ethers, podands, cryptands, spherands, calixarenes, cyclodextrins, cyclophanes, cryptophanes, carcerands and hemicarcerands., Host-Guest interactions, pre-organization and complimentarity, lock and key analogy. Binding of cationic, anionic, ion pair and neutral guest molecules.

Crystal engineering: role of H-bonding and other weak interactions.

Self-assembly molecules: design, synthesis and properties of the molecules, self assembling by H-bonding, metal-ligand interactions and other weak interactions, metallomacrocycles, catenanes, rotaxanes, helicates and knots.

Molecular devices: molecular electronic devices, molecular wires, molecular rectifiers, molecular switches, molecular logic.

Relevance of supramolecular chemistry to mimic biological systems: cyclodextrins as enzyme mimics, ion channel mimics, supramolecular catalysis etc.

Examples of recent developments in supramolecular chemistry from current literature

Reference Books:

1. J. -M. Lehn; Supramolecular Chemistry-Concepts and Perspectives (Wiley-VCH, 1995)
2. D. Beer, P. A. Gale, D. K. Smith; Supramolecular Chemistry (Oxford University Press, 1999)
3. W. Steed and J. L. Atwood; Supramolecular Chemistry (Wiley, 2000)

Course name: Subject Paper (Transition Metal-Catalyzed Cross Coupling Reactions)
Course code: PHD/SP-04; Credit: 4
Lecture: 40

1. Simple guide to the stability of transition metal complexes.
2. Late transition metal catalysts (*e.g.* Pd, Pt, Ir, Rh, Ru, Ag, Au, etc), 3*d*-transition metal catalysts (*e.g.* Fe, Co, Ni, Cu, etc)
3. Role of ligands, bases, additives, solvents, etc.
4. Energy source: Heat, microwave, sound, light, etc.
5. Homogeneous catalysts, heterogeneous catalysts, metal-nanoparticles (MNPs) catalysts.
6. Basic steps involve in transition metal-catalyzed reactions.
7. Basic chemistry of Pd, Pd(0) and Pd(II) complexes, Pd (0) is the most widely used in homogeneous catalysis.
8. Type of organic substrates.
9. Coupling reactions: Heck (Mizoroki-Heck) coupling, Assymetric Heck reaction, Suzuki (Suzuki-Miyaura) coupling, Sonogashira coupling, Negishi coupling, Chan-Lam coupling, Buchwald-Hartwig reaction, Role of Ligands its influence in Buchwald-Hartwig coupling reaction.
10. Application of transition metal-catalyzed cross coupling reactions.

Reference Books:

1. Palladium Reagents and Catalysts, New Perspectives for the 21st Century- J. Tsuji (2003)
2. Organic Chemistry, Oxford University Press., J. Clayden, N. Greeves, S. Warren and P. Wothers
3. Principles and applications of organotransition metal chemistry- J.P. Collman, L.S. Hegsdus, J.R. Nortan and R.G. Finke.
4. The Organometallic chemistry of the transition metals, R.H. Crabtree
5. Metallo-organic chemistry, A.J. Pearson
6. Some Modern Methods of Organic Synthesis, W. Carruthers
7. Organic Synthesis via Boranes, H. C. Brown

Course name: Subject Paper (Application of NMR Spectroscopy in Modern Research)
Course code: PHD/SP-04; Credit: 4
Lecture: 40

1. 1D NMR: ^{1}H, ^{11}B, ^{13}C, ^{15}N, ^{17}O, ^{19}F, ^{29}Si, ^{31}P, ^{51}V, ^{57}Fe, and ^{195}Pt NMR spectroscopy. Homo and Heteronuclear coupling. 1st order and 2nd order spectra. AB, ABX, AMX, AB_n etc, types of coupling in ^{1}H NMR.
2. 2D NMR: Homonuclear: COSY, DQF COSY, NOESY, ROESY, TOCSY, INADEQUATE Heteronuclear: HETCOR, HMBC, HMQC, HOESY
3. Application of NMR in identification of organic (including Natural products, Proteins), organometallic and inorganic compounds, understanding of molecular dynamics as well as mechanism and kinetics of reactions.
4. MRI technique and its applications.
5. Solid state NMR.

Reference Books:

1. Introduction To Spectroscopy- Pavia, lampman, Kriz, Vyvyan
2. Structure Elucidation by NMR in Organic Chemistry – Eberhard Breitmaier
3. A Complete Introduction to Modern NMR Spectroscopy – Roger S. Macomber
4. Biological NMR Spectroscopy – J. L. Markley, S. J. Opella
5. NMR and Chemistry – Dr. J. W. Akitt, Professor B. E. Mann
6. NMR Data Interpretation Explained – N. E. Jacobsen
7. NMR Basic Principles and Progress: Solid state NMR - P. Diehl E. Fluck H. GUnther R. Kosfeld J. Seelig
8. 50 and More Essential NMR Experiments – M. Findeisen, S. Berger

Course name: Subject Paper (Study of Structure and Function of Nucleic Acids and Proteins)
Course code: PHD/SP-04; Credit: 4
Lecture: 40

1. Primary secondary and tertiary structure of DNA, RNA and proteins.
2. Methodology and instrumentation for the isolation, sequencing and multiplication of DNA. Methodology and instrumentation of determination of structure of DNA and RNA.
3. Methodology and instrumentation for the isolation, sequencing and crystallization of protein.
4. Methodology and instrumentation of determination of structure of proteins.
5. Sequencing alignment and homology modeling of new protein sequence.
6. Functions of DNA, RNA and proteins in human body.

Reference Books:

1. RNA methodologies a laboratory guide by Md. Maidul Islam, Neoti Book Agency, New Delhi.
2. Physical Biochemistry: Applications to Biochemistry and Molecular Biology by David Freifelder
3. Methods in Modern biophysics, by B. Nolting
4. Introduction to Biophysical methods in Protein and Neucleic Acid research, by J.A. Glasel
5. Methods in Modern Biophysics by B. Nolting
6. Introduction to Biophysical Methods in Protein and Neucleic Acid Research by J.A. Glasel.

Course name: Subject Paper (Application of Statistical Data in Modern Research)
Course code: PHD/SP-04; Credit: 4
Lecture: 40

1. Statistical Data Treatment and Evaluation: Errors, Accuracy, Precision, Standard Deviation, Confidence.

2. Determination of the stoichiometry and the association constant between the host and guest molecule.

3. Lower Limit of Detection (LOD or limit of detection)

4. Analysis of Signal and Noise in Instruments:

5. An Introduction to Different Spectrometric Methods for the analysis of compounds

Reference Books:

1. Fundamentals of Analytical Chemistry- Douglas A. Skoog, Donald M. West, F. James Holler and Stanley R. Crouch.
2. Instrumental Analysis- Douglas A. Skoog, F. James Holler and Stanley R. Crouch.

Course name: Subject Paper (Strategies and Trends in Advanced Organic Synthesis)
Course code: PHD/SP-04; Credit: 4
Lecture: 40

1. ***Design of Organic Synthesis***

Synthetic strategies: Introduction, target selection, terminology, aims and objectives, retro synthetic analysis, functional group interchange, disconnection synthons, synthetic equivalent transform, C-C disconnection, one group C-C disconnection, two group disconnections, 1,2-, 1,3-, 1,4-, 1,5-, 1,6-difunctional compounds, applications of some important strategies in organic synthesis, chemoselectivity, regioselectivity, stereoselectivity, cyclisation reactions (3 to 7 membered rings), reversal polarity, consecutive and convergent synthesis, some selected synthesis.

2. ***Emerging greener methodologies***

Basic principles of Green Chemistry and their illustrations with examples, prevention of waste/by-products, prevention/Minimization of hazardous/toxic products, atom economy, Designing safer chemicals - different basic approaches, selection of appropriate auxiliary substances (solvents, separation agents etc).

Examples of green synthesis/reactions: Green starting materials, green reagents, real world cases (traditional processes and green ones).

Future trends in Green Chemistry: OHSA rules, biomimetic, multifunctional reagents; combinatorial green chemistry; proliferation of solvent less reactions; noncovalent derivatization.

Green solvents: Aqueous medium: Enhancement of selectivity, efficiency, and industrial applicability, ionic liquids, supercritical fluids, solvent free neat reactions in liquid phase, solvent

free solid phase reactions.

Nonconventional energy sources: microwave assisted reaction, ultrasound assisted reactions, photochemical reactions using sunlight.

Green catalysis: Heterogeneous catalysis: Use of zeolites, silica, alumina, clay, polymers, cyclodextrin, and supported catalysts; Biocatalysis: enzymes, microbes; Phase-transfer catalysis.

Reference Books:

1. Organic Synthesis, Michael B. Smith. 2nd Edition, McGraw Hill, 2005.
2. Some modern methods of organic synthesis, W. Carruthers, 3rd Edition, Cambridge University Press, 2001.
3. Organic Synthesis, The disconnection Approach, S. Warren, Wiley India Edition, John Wiley & Sons, 2007.
4. Organic Chemistry, Clayden, Warren and Wothers. Oxford University Press 2001.
5. New trends in green chemistry: V. K. Ahluwalia, M. Kidwai, New Age Publications, 2004.
6. Green Chemistry: Theory and Practice. P.T. Anastas and J.C. Warner. Oxford University Press, 2000.
7. Green Chemistry: Introductory Text. M. Lancaster Royal Society of Chemistry (London), 2010.

Course Name: Subject Paper (Chemistry of Nanomaterials)
Course Code: PHD/SP-04; Credit: 4
Lecture: 40

1. History of Nanoscience, Nano-world definitions, Properties of Nanomaterials,
2. Typical synthetic strategies for nanomaterials: Chemical routes, Electrochemical methods, Vapor growth Thin films methods: chemical vapor deposition, physical vapor deposition (sputtering, laser ablation), Langmuir-Blodgett growth Mechanical methods: ball milling, mechanical attrition Sol-gel methods Special nanomaterials: carbon nanotubes, fullerenes, nanowires.
3. Modern characterization methods: Scanning and Transmission Electron Microscopy, Scanning Probe Microscopies: Atomic Force, scanning tunneling microscopy, Diffraction and scattering techniques, Vibrational spectroscopy, Surface techniques
4. Applications of nanomaterials in different areas: Nano-bio interaction and nanomaterials as a drug delivery agent. Nano-electronics, Photovoltaic, fuel cells, batteries and energy-related applications, High strength nanocomposites, Nanoenergetic materials

Reference Books

1. N. R. Rao, A. Müller, A. K. Cheetham, The Chemistry of Nanomaterials: Synthesis, Properties and Applications.
2. B. P. Houdy and M. Lahmani, Nanomaterials and Nanochemistry, Springer, London, 2006.
3. P. Bréchignac, Houdy, M. Lahmani, Nanomaterials and Nanochemistry, Springer, London, 2006
4. The Physics and Chemistry of NanoSolids by Frank J. Owens and Charles P. Poole Jr, Wiley-Interscience, 2008.

Course Name: Subject Paper (Fluorescence Sensing)
Course Code: PHD/SP-04; Credit: 4
Lecture: 40

1. Spectral observable for fluorescence sensing, Mechanism of sensing, Sensing by collisional quenching , Energy transfer sensing, pH sensing
2. Photoinduced Electron Transfer (PET)
3. Probes for analyte recognition

Reference Books

1.Lakowicz, J. R. 1995, Advances in Fluorescence Sensing Technology II, Proc. SPIE 2388
2. Thompson, R. B. 1997,Advances in Fluorescence Sensing Technology III, Proc. SPIE 2980
3. Szmacinski, H. and Lakowicz, J. R., 1994, Topics in Fluorescence Spectroscopy, Volume 4, Plenum Press, New York.