SYLLABUS

For

Ph.D. Coursework in

CHEMISTRY

(CBCS format)

(Effective from the academic session 2019 – 2020 and onwards)

DEPARTMENT OF CHEMISTRY

BANKURA UNIVERSITY

BANKURA

Annexure-I

Ph.D. Course Work in Chemistry

Course Structure

Paper	Course Code	Course name (Core/Elective)	Marks (Credits)	Lectures per week
Compulsory Paper (CP)				
I	(Part A)	Research Methodology	50 (2)	4 hrs
	(Part B)	Computer Applications	50 (2)	
		Total	100 (4)	
Elective Paper (EP)				
II	CHEM-EP-1 (Part A)	Elective Paper	50 (2)	2 hrs
	CHEM-EP-2 (Part B)	Project work/Term Paper	50 (2)	
		Total	100 (4)	

Important Points to Note:

1. Duration of Course Work: One Semester (6 Months).
2. Total Marks: 200 (8 credits) (Two papers 100 marks each)
3. Students are required to secure minimum 75% attendance (as per university rules) in each course to qualify for appearing in End semester examination.
4. For **Paper – I** (Part A and Part B each), Marks 100, Examination time: 4 hrs
5. Each student has to study an elective paper of 2 credits.
6. For **Paper – II** (Part A), a student can opt any one of the elective course of his/her area of research interest. The elective papers shall be offered from Annexure - II depending upon the availability of the expert faculty. Marks 50, Examination time: 2 hrs) and for **Paper–II** (Part B), students have to submit a written report based on his/her **Review Work or Research Topic or Research Paper** under the supervision of his/her respective supervisor and finally one presentation should be given using Power Point on same topic.

Annexure-II

Detailed Syllabus

Paper – I [Compulsory Paper (CP)]

Part A: Research Methodology (CHEM-CP-1): [Total 25 Lectures, 50 marks]

A1. Introduction to Research Methodology:
Meaning of Research, Objectives of Research, Motivations in Research, Types of Research, Criteria of good Research, What is Research Problem? Basic and Applied research.

A2. Review of Literature and Literature survey:
Meaning and Purpose of the Literature Review & Literature Survey, Identification of the related Literature.

A3. The Research Report:
General format of the Research report, style and formatting of writing, typing of the research report.

A4. Testing of Hypotheses and Sampling design:
Definition, Concepts Concerning Testing of Hypotheses, Formulation of hypotheses and related difficulties; Needs of sampling, Sampling for chemical analysis, Random sampling

A5. Quantification of research output:
Impact Factor, *h*-index, *i10*-index and *i20*-index, G-index.

A6. Ethics in Research and Intellectual Property Rights:
Environmental Impacts, Ethical Issues, Reproduction of published material, Plagiarism, Citation and Acknowledgement, Reproducibility and accountability.Intellectual Property Rights, Patents, Copyright, Royalty.

Part B: Computer Applications (CHEM-CP-2): [Total 25 Lectures, 50 marks]

B1. Computer Applications in Research: Literature survey using web, handling search engines.

Preparation of-

(i) Research papers: Using word processing software – MS Word/Latex/others,
(ii) Drawing graphs and diagrams – Origin/Excel/others,
(iii) Seminar presentations – Power point for oral and poster presentations,
(iv) Data presentation,
(v) Figure insertions in documents.

References:

1. C R Kothari, Research Methodology: Methods and Techniques, New Age International (P)Ltd. (2010) , New Delhi
2. Garg, B.L., Karadia, R., Agarwal, F. and Agarwal, U.K., 2002. *An introduction toResearch Methodology*, RBSA Publishers.
3. Handbook of Communication and Social Interaction Skills by John O. Greene, Brant Raney Burleson.

4. W.M.K.Trochim, 2005. *Research Methods: the concise knowledge base*, AtomicDog Publishing. 270p.
5. Ranjit Kumar, Research Methodology: A Step-by-Step Guide for Beginners, SAGE Publications
6. Inderpal Singh, Research Methodology and Statistical Methods, Kalyani Publishers, Ludhiana.
7. G Kanji 100 statistical tests, Sage Publications.
8. R.A. Day (1992) How to write and publish a scientific paper. Cambridge Universitypress.London.
9. P.K. Sinha (1992). Computer Fundamentals, BPB Publications, New Delhi.
10. SPSS – Operating Manual and handbook – Latest version.
11. Leon & Leon (2002). Internet for everyone, Vikas Publishing House.

Paper – II [Elective Paper (EP)]

Part A: Elective Paper (CHEM-EP-1): [Total 25 Lectures, 50 marks]

Student can opt any one of the following elective paper of his/her area of research interest

Course Name: Application of Modern characterization Techniques
Course Code: CHEM-EP-1.1
Full Marks: 50
Credit: 2
Course Contents:

Ultraviolet Spectroscopy: Introduction. Studies of conjugated and extended conjugated systems etc. Woodward rules. Spectrophotometry, theory and applications.

Infrared Spectroscopy: Introduction. Identification of functional groups, hydrogen bonding etc., metal ligand vibrations.

Nuclear Magnetic Resonance Spectroscopy: Introduction. Application of ^{1}H and ^{13}C NMR spectroscopy techniques in the structural determination of complex organic systems.

Mass Spectrometry: Basic concepts. Fragmentation and rearrangements (including McLafferty rearrangement) of different classes of organic molecules. Isotope effects etc.

Structural elucidation by joint application of UV, IR, NMR and mass spectrometry

Electron Spin Resonance Spectroscopy: A brief review of theory. Analysis of ESR spectra of systems in liquid phase, radicals containing single set, multiple sets of protons, triplet ground states. Transitionmetal ions. Rare earth ions, ion in solid state. Double resonance techniques: ENDOR in liquid solution, ENDOR in powers and non-oriented solids. Biological applications: Substrate free radical, flavins and metal free flavin proteins, photosynthesis, Heme proteins, Iron-sulphur proteins, spin labels.

Fluorescence spectroscopy: Fluorescence energy transfer and its applications to measurement of distances in molecules.

Reference:

1. R. L. Pecsok, L. D. Shields, T. Cairns and L.C. Mc William, Modern Methods of Chemical Analysis, 2nd Edition (1976), John Wiley, New York.

2. Robert M. Silverstein, Francis X. Webster, David Kiemle, Spectroscopic identification of organic compounds, John Wiley & Sons; 7th Revised edition 2005.
3. G. D. Christian, Analytical Chemistry, 5th Edition (1994), John Wiley & Sons, New York.
4. D. A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, Analytical Chemistry - An Introduction, 7th Edition (2000), Saunders College Publishing, Philadelphia, London.
5. G. M. Barrow, Introduction to Molecular Spectroscopy, (1962) McGraw-Hill.
6. C. N. Banwell and E. M. McCash, Fundamentals of Molecular Spectroscopy, 4th edition, (1994), Tata McGraw Hill, New Delhi.
7. J. M. Hollas, Modern Spectroscopy, 4th edition (2004), John Wiley & Sons, Ltd., Chichester.
8. W. Kemp, *Organic Spectroscopy*, 3rd Edn, Macmillan Press Ltd., 1991.

Course Name: Catalysis: Theory, Synthesis, Characterization and application
Course Code: CHEM-EP-1.2
Full Marks: 50
Credit: 2
Course Contents:

Adsorption, Types of adsorption and Catalysis, Adsorption Kinetics, law of mass action, conversion, yield, selectivity, reaction rate, activation energy, kinetic orders, molecularity, rank, power rate law

Synthesis of Catalyst. In-situ polymerization and composite formation (IPCF) reaction. Homogeneous and Heterogeneous catalysis.

Characterization by Powder X-ray diffraction technique, Scanning Electron Microscope (SEM) and Transmission Electron Microscope (TEM).

Terminology in catalysis, TO(Turnover), TON(Turnover number), TOF(Turnover frequency).

Sequences involved in a catalysed reaction, other terms used in catalysis, enantioselectivity, stereoselectivity, chemoselectivity, regioselectivity, Asymmetric synthesis using a catalyst. Sensor. Synthesis of Metal-catalyst (Pd, Ru, Cu and Fe) and their application in Sonogashira, Heck, Stille, Suzuki coupling and Click reaction.

Reference:

1. R. J. Farrauto& C. H. Bartholomew, Fundamentals of Industrial catalytic Processes, Blackie Academic & Professional, 1997
2. H. S. Fogler, Elements of Chemical reaction engineering, Prentice – Hall of India, 2002, Third edition.
3. J.J. Carberry, Chemical and catalytic reaction Engineering, Dover Publications, 2001
4. Chemistry of nanomaterials: Synthesis, properties and applications - CNR Rao et.al.
5. Nanoparticles: From theory to applications, Wiley Weinheim, 2004 - G. Schmidt.
6. The chemistry of nanomaterials: Synthesis, properties and applications, Wiley VCH VerlagGmbh& Co, Weinheim, 2004 - C.N.R.Rao, A. Muller, A. K. Cheetham (Eds).
7. D. Gupta, *Basic Organometallic Chemistry: Concepts, Syntheses and Applications*, Universities Press, 2011.
8. J. M. Thomas & W. J. Thomas, Principles and Practice of Heterogeneous Catalysis, VCH, 1997
9. J. M. Smith, Chemical Engineering Kinetics, McGraw-Hill Book Company, 1981

Course Name: Bioinorganic, Bioorganic and Electro Chemistry
Course Code: CHEM-EP-1.3
Full Marks: 50
Credit: 2
Course Contents:

Overview of Bioorganic Chemistry- Historical Connection Between Organic and Biological Chemistry; Weak Interactions in Organic and Biological World; Proximity Effect in Organic Chemistry; Molecular Recognition; Chemistry of the Living Cells; Analogy Between Biochemical and Organic Reaction. Nucleic acids, purine and pyrimidine bases, nucleosides, and nucleotides. Genetic code of life, replication, transcription and translation of DNA, genetic information transfer and heredity. Types of sugars, deoxy sugars, amino sugars and polysaccharides.

Occurrence and observation of tetrapyrrole ring in biology (Haemoglobin, myoglobin, cytochromes, chlorophyll, enzymes, Vitamin B12) and their activity. Model study. Example of metalloenzymes. Spin state of iron and its biological relevance. Experimental techniques for structural elucidation: MM, EPR, Mössbauer etc. Inorganic chemistry in medicine, platinum complexes, Mo=S complexes as anti-cancer drugs.

Activity coefficients of electrolyte solutions; Debye-Hückel-Onsager theory for electrical conduction in electrolyte solutions; limitation of Debye-Hückel-Onsager theory; Ion-atmosphere, Ion-solvent interaction, Enthalpy of Ion-solvent interaction and its calculation. Solvation and solvation number.

Reference:

1. Hermann Dugas: Bioorganic Chemistry-A chemical Approach to Enzyme Action; 3rd Edition.
2. The organic chemistry of enzyme-catalyzed reactions, by Richard B. Silverman, Academic Press, San Diego, 2000, 717 pp.
3. Principles of bioinorganic chemistry: By S J Lippard and J M Berg. pp 411. University Science Books, Mill Valley, California. 1994.
4. Bioinorganic Chemistry, By A. K. Das, Books & Allied (P) Ltd. Kolkata 2007.
5. Bioinorganic Chemistry, A Survey, By Ei-Ichiro Ochiai, 1st Edition, pp 360. Academic Press, Elsevier 2009
6. J.O'M Bockris, A.K.N Reddy and M.G. Aldeco, Modern Electrochemistry, Published by Springer.
7. Samuel Glasstone, An Introduction to Electrochemistry, East West Press Private, Limited

Course Name: Supramolecules, Natural products and Macromolecules
Course Code: CHEM-EP-1.4
Full Marks: 50
Credit: 2
Course Contents:

Fundamentals of Supramolecular Chemistry: Definition, History, Nature of supramolecular interactions.

Biomimetic systems and artificial receptors:

(a) Cation Binding Hosts -Podand, Crown Ether, Cryptand, Spherand; Nomenclature, Selectivity and Solution Behaviour; Alkalides, Electrides, Calixarenes and Siderophores.

(b) Anion binding hosts - Challenges and Concepts, Biological Receptors, Conversion of Cation Hosts to Anion Hosts, Neutral Receptors, Metal-Containing Receptors, Cholapods.
(c) Ion Pair Receptors - Contact Ion Pairs, Cascade Complexes, Remote Anion and Cation Binding Sites, Symport and Metals Extraction.
(d) Hosts for Neutral Receptors -Clathrates, Inclusion Compounds, Zeolites, Intercalates, Coordination Polymers, Guest Binding by Cavitands and Cyclodextrins, cucurbituril.
Alkaloids: Familiarity with methods of structure elucidation (chemical & spectroscopic method), synthesis and reaction of alkaloids (quinine, atropine, coniine and papaverine).Terpenoids: Structure elucidation,synthesis and reaction of Terpenoids (Abietic acid/ β-Carotene).
Structure, synthesis and reactions of steroids (cholesterol, testosterone, estrone, progesterone). Structure, synthesis and reactions of flavonoids and coumarins.Structure and synthesis of porphyrins (haemoglobin, chlorophyll). Structure and synthesis of prostaglandins (PGE2, PGF2α).
Introduction; Carothers' equation, average molecular weights and their determination; kinetics of addition and condensation polymerization, flexibility of polymer chain, statistics of polymer dimensions and configurations, effect of solvent on the average dimensions; theories of polymer solutions: excluded volume and Flory-Huggins theory.

Reference:

1. J. M. Lehn, Supramolecular Chemistry, VCH, Weinheim, 19951.
2. Supramolecular Chemistry by J. W. Steed & J. L. Atwood, 2nd Edn John Wiley, 2009.
3. Crystal Engineering**.** The Design of Organic Solids by G.R. Desiraju, Elsevier, 1989.
4. S. V. Bhat, B. A. Nagasampagi and M. Sivakumar, *Chemistry of Natural Products,* Narosa Publishing House, New Delhi, 2005.
5. S. P. Bhutani, *Chemistry of Biomolecules,* CRC Press, 2010.
6. X.-T. Liang and W.-S. Fang, *Medicinal Chemistry of Bioactive Natural Products,* John Wiley & Sons, 2006.
7. S. F. Sun, *Physical Chemistry of Macromolecules: Basic Principles and Issues,* John Wiley & Sons, New York, 1994.
8. C. Tanford, *Physical Chemistry of Macromolecules*, John Wiley & Sons, Inc, New York, 1961.
9. P. Ghosh, *Polymer Science and Technology of Plastic and Rubber*, Tata McGraw-Hill Publishing Company Limited. 2008.

Part B: Elective Paper (CHEM-EP-2):

Students have to submit a written report based on his/her **Review Work or Research Topic or Research Paper** under the supervision of his/her respective supervisor and finally one presentation should be given using Power Point on same topic.