Course Structure of M. Phil. in Chemistry

(Effective from Academic Year 2019-20)

P.G. Department of Chemistry

North Orissa University, Baripada 757 003

EMESTER-I

Sl. No	Course Title	Course Code	Credit	Full Mark
1.	Research Methodology	CH-601	05	50
2.	General Theory	CH-603	05	50
3.	Practical	CH-605	10	100
Total			**20**	**200**

SEMESTER-II

Sl. No	Course Title	Course Code	Credit	Full Mark
1.	Elective-I (Techniques in Chemistry)	CH-602	05	50
2.	*Elective-II (Materials/Organic/Inorganic)	CH-604	05	50
3.	Project Dissertation	CH-606	10	100
Total			**20**	**200**

*M. Phil. Scholars shall present at least 01 no. of research paper (oral/poster) in a conference /seminar before submission of the dissertation for adjudication and produce evidence for the same in the form of presentation certificates.

*From Elective-II, the student can opt any one of the paper

ELECTIVE GROUPS

A. **Chemistry of Materials**
B. **Advanced Organic Chemistry**
C. **Advanced Inorganic Chemistry**

Programme Outcome:

- Gained knowledge about research, literature survey, scientific paper writing and communication
- Developing knowledge on green chemistry, organic photo chemistry, inorganic photo chemistry and supra molecular chemistry
- Gained knowledge on instrumental techniques for the analysis and characterization of synthesized compounds and prepared materials.

Programme Specific Outcome:

- Expected to gain basic knowledge on literature survey, scientific ethics and scientific writing
- Constructive analytical skill will be developed for studies on advanced research and industrial jobs
- Create a responsibility and awareness to maintaina safer laboratory practice and systematic documentation

SEMESTER-I

CH-601 **Marks- 50 (5 Credit)**

RESEARCH METHODOLOGY

OBJECTIVES:

The main objective of this course is to introduce the basic concepts in research methodology in chemical science. This course addresses the issues inherent in selecting a research problem and discuss the techniques and tools to be employed in completing a research project. This will also enable the students to prepare report writing, framing research proposals, develop research strategies, understand data collection, analysis of data and interpretation.

CONTENTS:

UNIT-I

Scientific Research: Definition, characteristics, types, need of research, Identification of the problem, assessing the status of the problem, formulating the objectives, preparing design (experimental or otherwise), Actual investigation, Determining the mode of attack.

UNIT-II

Literature Survey: Primary sources (Journals and Patents), Secondary resources (abstracts, CA, collective indexes, reviews, awareness service, general treatise, monographs on specific areas, reference books), Basic ideas of literature search on web (Scifinder, Scopus, Scirus, Science Direct), Citation index, Impact factor of research papers.

UNIT-III

Documentation and Scientific writing: Organization and writing of manuscript/paper, monographs, authored books and edited books, Thesis writing, Structure and Components of Research Report, Types of Report: research papers, thesis, Research Project Reports, Pictures and Graphs, citation styles, writing a review of paper, Bibliography.

UNIT-IV

Statistical Methods of Data Analyses: Fundamental of statistical analyses- types, mean, median, mode, range, variance, standard deviation, Test for rejection of outliers (Q test), Levels of confidence and significance, Test of significance (F-test, student T-test, paired T-test), Least square methods of fitting linear equations, (simple linear cases and weighted linear case), correlation coefficient and coefficient of determination.

UNIT-V

Computer Applications in Chemistry: Computer software and chemistry, Computer technique used in chemistry with special reference to UV-Visible spectroscopy, chromatography, mass spectroscopy, Applications of some computer packages (MS-Excel, Origin, Chem draw) to chemistry.

COURSE OUTCOMES:

On completion of the course the student will be able to

- Gained knowledge on basic research, scientific literature searching, and scientific documentation
- Learn about the statistical method of data analysis
- Gained knowledge how to apply computational calculations for use of chemistry
- Learn how to integrate the use of computer in different analytical instruments.
- Gained ability how to use different literature search data base

Books Recommended

1. Research Methodology - Methods & Techniques, C.R. Kothari, Wiley Easten Ltd. New Delhi 1985.
2. Research Methodology - A step by step Guide for Beginners 2nd edn. Kumar Ranjit, Pearson Education, Singapore, 2005.
3. Introduction to Research & Research Methodology. M.S. Sridhar.
4. Analytical Chemistry, G.D. Christian, 6th Edn, Wiley Student Edition.
5. Computer for Chemists, S.K. Pundir & A. Bansal, Pragati Prakashan 2008.
6. Nomenclature for the presentation of results of chemical analysis. (IUPAC Recommendations 1994) *Pure and Appl. Chem.*Vol.66, No. 3, pp.595-608,1994.
7. B.S. Furniss, A.J. Hannaford, P.W.G. Smith, A.R. Tatchell, Vogel's Text Book of Practical Organic Chemistry, 5th Edition, Pearson, New Delhi, 1989.

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CH-603 **Full marks – 50 (5 Credits)**

GENERAL THEORY

OBJECTIVES:

To objective of the course will be to understand the principles behind green chemistry, supramolecular chemistry, and photochemical reactions of some common organic and inorganic compounds. The course also gives an understanding of non-stochiometric oxides, structures, reactions of solids and thermal decomposition.

CONTENTS:

Unit-I

Green chemistry: Introduction, basic principles of green chemistry. Designing a green synthesis: Green starting materials, green reagents, green solvents and reaction conditions, green catalysts**.** Use of the following in green synthesis with suitable examples: a) Green reagents: dimethylcarbonate, polymer supported reagents. b) Green catalysts: Acid catalysts, oxidation catalysts, basic catalysts, phase transfer catalysts [benzyltrimethyl ammonium chloride (TMBA), Tetra-n-butyl ammonium chloride, crown ethers]. c) Green solvents: water, ionic liquids, supercritical carbon dioxide. d) Solid state reactions: solid phase synthesis, solid supported synthesis. e) Microwave assisted synthesis: reactions in water, reactions in organic solvents, solvent free reactions.

Unit-II

Supramolecular Chemistry: Concept of Supramolecular Chemistry, Different types of non-covalent interactions. Molecular receptors for neutral, cationic and anionic substrates. Co-receptors and multiple recognition, Introduction to self assembly with examples, Applications of Supramolecular Chemistry in transport processes and Catalysis.

Unit-III

Organic photochemistry: Introduction to photochemistry, photochemistry of carbonyl compounds (α,β cleavage and intramolecular H-abstraction), photorearrangements (cyclopentenone, cyclohexanone, dienones, β,γ unsaturated ketones and di-π-methane rearrangements). Alkenes (cis-trans isomerization and dimerization), conjugated dienes (cis-

trans isomerization, sigmatropic shifts, electrocyclic reactions and intramolecular 2+4 cycloaddition), Aromatic compounds (addition of alkenes to aromatic compounds).

Unit-IV

Inorganic photochemistry: Basic Photochemical Processes, Kinetic factors affecting quantum yields; photo-substitution, photo-redox and ligand photo reactions with special reference to Co (III), Rh (III) and Cr (III) complexes.

Unit-V

Solid state chemistry: Crystal defects, Non-stochiometry in oxides, Structure of ionic crystals (MX, MX_2, Spinel, Perovoskite type).

Reactions of solids: Classification, Thermal decomposition with examples and diffusion in solids: atomic approach.

COURSE OUTCOMES:

On completion of the course the student will be able to

- gain knowledge about the green and sustainable chemistry
- acquire in-depth idea about supramolecular chemistry
- gain the knowledge on sun light driven reaction of organic molecules as well as inorganic molecules
- acquire knowledge on solid state chemistry

Books Recommended

1. Supramolecular Chemistry, Paul D. Beer, Philip A. Gale, David K. Smith, Oxford Press.
2. Supramolecular Chemistry, Jonathan W. Steed and Jerry L. Atwood, 2nd Edition, Wiley.
3. Bioorganic, Bioinorganic and Supramolecular Chemistry, P.S. Kalsi, New Age.
4. Supramolecular Chemistry, J.M. Lehn,VCH.
5. Elements of Inorganic Photochemistry, G.J. Ferraudi, Wiley.
6. Principles of the Solid State, H.V. Keer, Wiley Eastern.
7. Photochemistry and Pericyclic Reactions, Jagdamba Singh and Jaya Singh, New Age International Publishers.

8. Solid State Chemistry, D.K. Chakrabarty, New Age International Publishers.

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CH-605 **Full marks – 100 (10 Credits)**

PRACTICAL

1. Determination of rate of base hydrolysis of oxalatopentammine cobalt(III) ion at varying concentration of alkali by titrametric and spectrophotometric methods.
2. Preparation of N,N'- bis(salicylaldehyde)ethylenediammine (salenH_2) and Co(Salen).
3. Determination of molecular weight of polymers by Ubbelhood Viscometer.
4. Determination of pH of a given solution by spectrophotometric method.
5. Synthesis of organic compounds involving two to three steps and various techniques like steam and vacuum distillation.
6. Isolation and purification of organic compounds by using TLC and PC.
7. Determination of indicator constant of methyl red spectrophotometrically.
8. Determination of solubility product of Silver chloride.
9. Determination of Phosphate ion in solution spectrophotometrically.

COURES OUTCOMES:

On completion of the course the student will be able to

- Prepare coordination complexes.
- Synthesize different organic molecules.
- perform TLC and column chromatography

Books Recommended

1. A Text Book of Quantitative Inorganic Analysis – A.I. Vogel, ELBS (India).
2. A Text Book of Quantitative Organic Analysis – A.I. Vogel, ELBS (India).

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SEMESTER II

ELECTIVE-I (Techniques in Chemistry)

CH-602 **Marks-50 (5 Credits)**

OBJECTIVES:

The objective of the course will be to introduce fundamental technological principles and applications of advanced characterisation techniques (e.g. X-ray, TEM, SEM, XPS, UV-visible-DRS, FTIR, photoluminescence, FT NMR) used to establish the physical and chemical properties of materials at the nanoscale. It is an amalgamation of the science behind these characterization techniques and their application in material systems.

CONTENTS:

Unit -I

X-ray techniques for materials characterization: X-ray diffraction: Principle, measuring system and application for characterization of powdered materials.

X-ray fluorescence: Principle, instrumentation and their applications for analysis of solid samples

UNIT-II

Microscopic Techniques: Principle, instrumentation and applications of Optical microscope, Scanning Electron Microscope (SEM) and Transmission Electron Microscope (TEM) with special reference to materials.

Unit-III

Surface characterization: Molecular kinetic picture of adsorption (physical and chemical), adsorption isotherms, surface acidity and basicity and their determination of titrametric and TPD (Temperature Progrmmed Desorption) methods.

Unit-IV

Spectroscopic methods-I: UV-Visible Diffuse Reflectance Spectroscopy: Principle, instrumentation and application to powder materials.

FT-IR spectroscopy: Principle, instrumentation and applications.

Mass spectroscopy: Introduction to soft ionization techniques and illustrative examples of macromolecular and supramolecular chemistry.

Unit-V

Spectroscopic methods-II (a) NMR: Theory of FT-NMR, quantum mechanical description of NMR, spin lattice relaxation, Bloch equations-nuclear induction, NOE advance concepts-pulse sequences, INEPT and DEPT cross polatization. Introduction to ^{31}P and ^{19}F NMR.

(b) ESR: Comparison between NMR and ESR, applications of ESR spectroscope ENDOR, ELDOR.

COURES OUTCOMES:

On completion of the course the student will be able to

- Acquire knowledge on principle and applications of different X-ray techniques such as P-XRD and XRF etc.
- Gained knowledge how to characterize the nanoscale materials using SEM and TEM
- Acquire knowledge on different spectroscopic techniques such as UV-Vis, FT-IR, NMR and Mass spectrometry

Books Recommended

1. Adsorption and Catalysis by D. K. Chakravortty
2. Adsorption by Powders and Porous solids: Principles, methodology and applications by F. Rouquerol, J Rouquerol and K. Sing, Academic Press (1999).
3. A practical guide to Instrumental Analysis, E. Pingor, CRC Press (1995)

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ELECTIVE-II (Group A: Chemistry of Materials)

CH-604 **Marks-50 (5 Credits)**

OBJECTIVES

This course focuses on the fundamental aspects of materials science and discusses on their synthesis, properties and specific applications and gives an understanding of materials, especially polymer matrix composites and carbon-carbon composites. The course also

focuses on unique properties of superconducting materials and biomaterials. The course is intended to give an overview of the fast growing field of biomaterials and their applications

CONTENTS:

Unit -I

Nanomaterials: Nanoscale regime and its importance, chemistry of nanomaterials, Size dependent physico-chemical properties, Forms of nanomaterials (e.g power, film/coating, composite, nanowires, nanotubes, nanopropus, nanocluster etc.), General physic-chemical methods of synthesis of nanomaterials (Plasma, electrodeposition, evaporation, condensation, coprecipitation, sol-gel, microemulsion methods) with examples. General applications of nanomaterials.

UNIT-II

Composite materials: Basic idea of composites, alloys, blending, matrixes and reinforcements materials, carbon-carbon composites, biocomposites, nanocomposites, fabrication of polymer composites, Processing of composites, interfaces and inter-phases in composites, environmental effect on composites; applications of composites.

Unit-III

Superconducting materials: Introduction, types of superconductors (conventional, organic, fullerenes and high temperature), thermodynamic relations, London equation, coherence length.

Applications of superconducting materials

Unit-IV

Biomaterials-I: Introduction to biomaterials, types of biomaterials and their applications. Biomineralisation: concept of mineralization processes (Nucleation and growth), biogenic minerals (like carbonate, phosphates and oxalates) with special reference to calcium.

Unit-V

Biomaterials-II: Introduction to biopolymers and their material applications: Cellulose, hemi cellulose and chitin.

Books Recommended

1. Polymer composites: Gupta and Gupta, New Age Publications
2. Nanochemistry: A chemical approach to Nanomaterials, RSC Publication, G A Ozin and A C Arsenault
3. Chemistry of nanomaterials, C. N. R. Rao.
4. Principle of Nanotechnology, G. Ali Mansoori, World Scientific (2005).

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ELECTIVE-II (Group B: Advanced Inorganic Chemistry)

CH 604 **Full Marks: 50 (5 Credits)**

OBJECTIVES

The objective of the course is to get a broad and in-depth idea about transition metal complex formation, theories and mechanism.

CONTENTS

UNIT-I

Crystal field theory: Octahedral and tetrahedral Crystal Field Potential and their effect on d-wave functions (Qualitative). Free ion terms wave function for d2-system. The effect of weak octahedral field on S, P, D, and F, terms (quantitative). Correlation Diagram for d2 system.

UNIT-II

Electronic Spectra of Complexes: Intensity & Broadening of Spectra: Spectra of Octahedral and tetrahedral complexes. Calculation of β and Dq and assignment of spectra for dn system.

UNIT-III

Inorganic Photochemistry: Basic photochemical process. Kinetic factors affecting quantum Yields. Photosubstitution, Photo-redox and ligand photo reactions with special reference to, Co(III), Rh(III), and Cr(III) complexes.

UNIT-IV

Mechanism of Reactions of Coordination Compounds in Solutions: Mechanism of substitution reaction at the Cr(III), Pt(II) Centre in comparison with CO(III) Trans effects. Substitution of Fe(III) and the proton ambiguity. Kinetics of Chelate formation**.** Redox-

reactions, inner-sphere and outer-sphere electron transfer. Marcus cross relationship from thermodynamics. Application of the Marcus cross relationship.

UNIT-V

Heme Iron proteins-cytochromes, with special reference to cytochrome -C, Non Heme Iron proteins as electron carriers: Rubredoxin and ferridoxin. Vitamin B 12 - Structure and reactivity inorganic Chemistry of Vitamin B 12 model compounds.

OUTCOMES:

- Able to know the reaction mechanism of inorganic complex
- Got knowledge in bioinorganic chemistry
- Able to know the details of inorganic photochemistry

Books Recommended

1. Inorganic Chemistry: W. W. Perterfield (Addition Wesley Publishing Co.)
2. Rection Mechanism of Inorganic and organometallic Systems-R. B. Jordan(Ch. 7), (Oxford Press, N. Y. 1991)
3. Ligand Field Theory- B. N. Figgis
4. Physical Methods in Chemistry –R. S. Drago
5. Inorganic Reaction Mechanism -Basolo and Pearson.
6. Advanced Inorganic Chemistry - Cotton and Wilkson.
7. Inorganic Reaction Mechanism - R.O. Wilkins

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ELECTIVE-II (Group C: Advanced Organic Chemistry)

CH 604 **Full Marks: 50 (5 Credits)**

OBJECIVES:

The objective of the course is to understand the concept of Stereochemistry of organic molecules and their effect on reactivity as well as synthesis of drug molecules including heterocycles.

CONTENTS:

UNIT-I

Structure and Reactivity: Effect of structure on reactivity, Hammett equation (Linear Free Energy Relationship), Taft equation, substituent constants, Reaction constants, Application

of the concept of Linear free energy relationship in the determination of organic reaction mechanism. The HSAB (Hard Soft Acid Base) principle and simple illustration of its application in organic Chemistry such as those with reference to stability of organic compounds, symbiosis, nucleophilic reactivity. Effect of Conformation on reactivity with suitable examples.

UNIT-II

Asymmetric Synthesis: Introduction, Chiral auxiliaries, Enantiomeric excess, Chiral reagents, Chiral catalysts, Asymmetric hydrogenation, Methods of improvement of enantiomeric excess such as recrystalization, Asymmetric epoxidation, Asymmetric dihydroxylation, Enantioselectivity in the Sharpless Asymmetric dihydroxylation

UNIT-III

Heterocyclic Chemistry: Nomenclature and familiarity with heterocyclic ring systems (3-7 membered) containing up to three hetero atoms. Chemistry of pyrazole, imidazole, Oxazole, sydnones, azing pyridazines, pyrimidines, pyarazines, azepines, oxazines.

UNIT-IV

Organo-main-group Chemistry: Phosphorous, Sulfur, and Silicon: Phosphorous containing reagents, Reactions of phosphorous ylides, Stereoselectivity in Wittig and Wadsworth-Emmons reactions, Application of phosphorous reagents for the preparation of aldehydes, synthesis of alkenes from 1,2-diols, reductive cyclization of nitro compounds and conversion of alcohols into halides, Reactions of sulphur ylides with carbonyl compounds and dimsyl anions, rearrangements using sulphur ylides, use of dithioacetal for polarity reversal, Julia reactions, Peterson reaction, Use of silicone for the inversion of configuration of alkene, β-carbon stabilization.

UNIT-V

A General Study of the following Classes of Drugs

(1) Duretic and Cardiac drugs.

(2) Histamines & antihistaminic agents.

(3) Analgesic & antiviral agents.

(4) Antifertility drugs.

OUTCOMES:

On completion of the course the student will be able to.

- Illustrate the reaction mechanism aspects in the context of addition, elimination and substitution reaction.
- Assess the structural effects of organic molecules and functional groups on the tendency to participate in various types of organic reactions.
- Describe the methods of asymmetric synthesis which involve chiral substrate, chiral reagents, chiral auxiliary and chiral catalyst.
- Understand the mechanism of drug synthesis
- Get a job in pharmaceutical industry, agrochemicals and fine chemicals industry.

Books Recommended

1. Physical organic chemistry by Neil s. Issacs, Longman Scientific & Technical (1987)
2. Reactivity in Organic Chemistry by G.W. Klumpp. Wiley interscience Publication(1982)
3. Hand book of Heterocyclic Chemistry ,Alan R. Katritzky, Pergamon press(1985)
4. Heterocyclic Chemistry by T.L. Gilchrist ,Pitman Publishing Ltd.(1985)
5. Heterocyclic Chemistry by Joule & Smith, Van Norstand Reinhold (1989)
6. Organic Synthesis : The role of Boron & Silicon (Oxford Chem. Primer) S.E. Thomas. Oxford science publication
7. Medicinal & Pharmaceutical Chemistry. Harkishan singh & V.K. Kapoor. Vallabh Prakashan (1996).
8. Organic Chemistry, Clayden, Greeves, Warren, Wothers, Oxford Publications
9. Principles of Organic Synthesis by R.O.C. Norman, J. M. Coxon by CRC Press

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CH-606 **Marks-100(10 Credits)**

PROJECT DISSERTATION

Each student has to submit dissertation of the project work before the commencement of Semester-II examination.

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