COURSES OF STUDY

FOR THE

M.PHIL.EXAMINATION

IN

CHEMISTRY

Semester Pattern

(with effect from 2020-2021 session)

POST GRADUATE DEPARTMENT OF CHEMISTRY
UTKAL UNIVERSITY
VANI VIHAR, BHUBANESWAR

PREFACE

The Master of Philosophy (M.Phil.) in Chemistry course is designed primarily for post graduate students who intend to pursue higher studies in chemistry. It aims at enhancing the capacity of scholars and provides a platform for further research.

PROGRAMME OBJECTIVES:

- To accumulate basic knowledge on different aspects of research methodology.
- To impact advance knowledge of chemistry in different subjects which are required to understanding philosophy of chemistry.
- To train the post graduates capable of undertaking higher level chemical research.
- To produce skilled postgraduates who can act in the increasingly wide research area of chemistry.
- To practice innovative teaching methods to communicate clearly and effectively, orally and in writing.

PROGRAMME OUTCOMES:

1. The students will develop knowledge and understand the current issues, research and developments.
2. M.Phil students shall get new ideas about the current scenario by studying literature.
3. The scholars will acquire knowledge in soft skill and it can be introduced for class room teaching.
4. Improved the numerical aptitude and computational knowledge in the basic of collection and presentation of data.

P.G.DEPARTMENT OF CHEMISTRY
UTKAL UNIVERISTY
M.PHIL. SYLLABUS

COURSE STRUCTURE

M. Phil in Chemistry shall comprise two semesters, having total of 400 marks and 24 credits. There shall be two theory papers in each semester, General Theory and Elective in Sem.-I and Sem.-II respectively. Besides this Sem.-I and Sem.-II will have Seminar and Dissertation respectively.

SEMESTER –I

Course Code	Course Title	Credit	Marks
CH-601	Research Methodology	3	50
CH-603	General Theory-I	3	50
CH-605	General Theory-II	3	50
CH-607	Seminar	3	50

SEMESTER –II

Course Code	Course Title	Credit	Marks
CH-602	Elective-I (Organic/Physical./Inorganic)	3	50
CH-604	Elective-II (Organic/Physical./Inorganic)	3	50
CH-606	Dissertation	6	100

Total Credit: 24 **Total Marks: 400**

Regulations

Questions will be set unit wise and each unit will have subunits, in order to accommodate alternatives. The question will be set both subjective as well as short answer types. Pass mark in theorypapers is 50% in aggregate &for other papers (Seminar & Dissertation) the pass mark is 50% in individual papers.

SEMESTER –I

CH-601 **Marks- 50**

RESEARCH METHODOLOGY
(Unit Pattern)

Objective:

1. To understand the principles of research, literature survey and develop writing and presentation skills
2. To gain some knowledge about the applications of computer in Chemistry.

Outcome:

1. The students will know the different routes to design a research problem
2. Improved the competency in literature search, analysis and presentation of data, writing skills.
3. Improved the numerical aptitude and computational knowledge
4. Use of differetn computer softwares for collection of data and analysis.

UNIT- I

Introduction to research, Objective of research, types of research, significance of research, Research methods vs. methodology, research processes, formulating research problem, criteria of good research, ethics in research.

Reporting practical and project work, organizing a poster display and oral presentation.

Scientific writing

Writing scientific papers, justification for scientific contributions, bibliography, description of methods, conclusions, the need for illustration, style, publications of scientific work, writing ethics, avoiding plagiarism, writing of thesis, patent law, filing of patent.

Literature survey-I

Print resource: Primary sources (Journals and patents), Secondary resources (abstracts, CA, Beilstein, compendia and tables of information current contents, collective indexes, reviews, awareness service, general treatise, monographs on specific areas, reference books),

UNIT- II

Literature survey-II

Web resources, Journal access through web – Digitized and digital formats, E-journals, E-books, E-consortium, UGC infonet, Online and Digital libraries, Useful web links: Scifinder, Scopus, Scirus, Science Direct. Citation index, Impact factor, H-index, Internet discussion groups and communities, Blogs, Preprint servers, Sharing documents online, Report writing using templates, Online submission system, Tracking manuscript status, End-note and SciProof, Digital object identifier (DOI), Hot articles.

UNIT- III

Computer applications in chemistry

Computer Softwares and chemistry, Computer technique used in chemistry with special reference to UV-Visible spectroscopy, chromatography, mass spectroscopy, crystallography. Basic idea on computer use in drug discovery, chemical information, structure elucidation, synthesis design, simulation of reaction, physicochemical data, molecular modeling, molecular graphics, data banks.

Books Recommended:

1. Research Methodology – Methods & Techniques, C.R. Kothari, Wiley Eastern 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. Matthias Otto, Chemometrics – Statistics and Computer Applications in Analytical Chemistry, Wiley – VCH, 1999.
5. S.K. Pundir and A. Bansal Pragati, Computer for Chemists, S.K. Pundir and A. Bansal PragatiPrakashan 2008.
6. G.Grant and W. Richards, Computational Chemistry, Oxford University press.

CH-603 **GENERAL THEORY-I** **Full Marks -50**

Objective:

1) To introduce basic of quantum chemistry, macromolecular chemistry, molecular spectroscopy.
2) To study the thermodynamic behaviors of polymers in solutions
3) To study the solubility and solubility parameters, nature of crystallinity, effects of radiation on polymers and cross-linking of polymers.

Outcome:

1) Students will gain the knowledge of different types of spectra obtained experimentally.
2) Understand the structure and properties of polymer molecules and macro molecular compounds.
3) Understand about structure, thermodynamic properties and applications of some commercial polymers

Unit-I QUANTUM CHEMISTRY:

a) Application of Schrodinger's equation to the motion of electron in continuous and discontinuous potential field. Tunneling effect.
b) Angular Momentum: AM operators, Commutation relations, Ladder operations, Matrix from of AM operators, Elgen values and eigen functions for AM operators. Electron spin and antisymmetry principle.
c) Approximate Methods:-Perturbation theory for non-degenerate and degenerate states, Variation method: Application to Helium atom(by both the methods).Anharmonic oscillator and non-rigid rotator(by perturbation method)

Books:
1. Quantum Chemistry - Eyring,Walter,Kimball
2. Quantum Chemistry - A.K.Chandra
3. Quantum Chemistry - I.L.Pilar
4. Quantum Chemistry - R.K.Prasad

Unit-II MACROMOLECULAR CHEMISTRY:

Thermodynamics of polymer solutions: Basic concept of theory of solution & Criteria of Polymer solubility, Flory-Huggins Theory, Statistics of Polymer Chains: Random-flight chain model, Freely-rotation chain model, Hindered rotation model, Rational isomeric state model, Properties of Commercial Polymers: LDPE,HDPE, Polystyrene, Acrylic Polymers, neoprene, Fluorocarbon polymers, polyamides, thermosetting resins, polycarbonates.

Books:
1. A Text Book of Polymer Science - F.W.Billmyer
2. Physical Chemistry of Polymers – A.Tagar
3. Polymer Science & Technology of Plastic & Rubbers – P.Ghosh, Tata Mc.Graw Hill Co.Ltd. New Delhi
4. Organic Polymer Chemistry –K.J.Saunders.
5. Fundamentals of Polymer Science & Engineering – Anil Kumar &S.K.Gupta, TataMc.Graw Hill Co.Ltd. New Delhi
6. Polymer Science –Gowariker, Viswanath & Sreedhar

UNIT-III MOLECULAR SPECTRA:

a) Molecular Vibrations: Normal coordinates normal vibrations and vibrational energy. Nature and classifications of normal vibrations. The method of extreme field, overtones, combination bands and hot bands, coriolis interactions. Accidental degeneracy.
b) Vibration – Rotation Spectra: Linear molecule, vibrational and Rational Raman spectra. Effect of nuclear spin, polarization of Raman lines.
c) Applications of Molecular spectra: Determination of inter-nuclear distance, force constants, characteristics band frequencies.

Books:

1. Molecular spectroscopy - P.S.Sindhu
2. Group Theory - F.A.Cotton
3. Theoretical Chemistry - S.Glasstone
4. Modern Spectroscopy - J.M.Hollas

CH-605 **GENERAL THEORY-II** **Full Marks -50**

Objective: To introduce the advance concept of organometallic chemistry, catalysis, role of frontier orbitals in organic reaction and NMR spectral analysis of organic compounds.

Outcome: Students will acquire comprehensive knowledge on synthesis and applications of organometallic compounds, participation of FMO in organic reactions and interpretation of NMR spectra.

UNIT-I ORGANOMETALLIC CHEMISTRY AND CATALYSIS:

(A) Sigma (σ) and pi(π)-bonded organometallic compounds,Olefin acetylene complexes, metallocenes and Sandwich bonded Organometallics.

(B) Catalysis by organometallic compounds – Polymerization,alkane metathesis and isomerisation,alkane hydroformylation and reduction.

(C) Fluxional behavior of organometallic compounds.

(D) H M O Theory :
H M O approximations, symmetry factoring of Secular equations.
H M O Theory for benzene and Napthalene using symmetry rules.

UNIT-II

FRONTIER ORBITALS & ORGANIC CHEMICAL REACTIONS:

Introduction,Molecular Orbitals & Frontier Orbitals (HOMO & LUMO).Equation for estimating chemical reactivity,Ionic reactions,Principle of HSAB,Ambident nucleophiles & electrophiles, the a-effect. The anomeric effect,Thermal Pericyclic reactions, The Woodward-Hoffmann rules,Rates of Cycloaddition reactions,Energies & Coefficients of the frontier Orbitals of Dienes & dienophiles. Regioselectivity in Diels Alder reactions & 1,3 dipolar Cycloaddition,Periselectivity in pericyclic reactions. Discussion of the above items with suitable examples.

UNIT-III

NMR –Chemical Shift,spin-spin coupling,Relaxation mechanism,structural elucidation of organic compounds on the basis of ^{1}H and ^{13}C spectra.

Books :

1. Molecular Spectroscopy by – P.S.Sindhu
2. Introduction to Magnetic resonance - A.Carrington and A.R. M.C.Lachlan
3. Advanced Inorganic Chemistry – Cotton and Wilkinson (4^{th} Ed.)
4. Inorganic Chemistry – Huheey (3^{rd}Edn.)
5. Inorganic Chemistry – Perterifield

CH-607 **SEMINAR** **Full Marks -50**

Objective: To learn to develop review articles on a particular topic.

Outcome: Students will learn the way to present a research topic.

Student is required to present seminar on topic of his interest with a copy of the synopsis of the presentation.

SEMESTER –II

CH 602 **ELECTIVE-I** **Full Marks: 50**

ORGANIC CHEMISTRY-I

Objective: To make familiar with advanced topics of organic chemistry.

Outcome: Students will be more focused and get advanced concept of heterocyclic chemistry with respect to synthetic methodology and applications. .

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

HETEROCYCLIC CHEMISTRY:

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

UNIT-III

SYNTHETIC METHODOLOGY IN ORGANIC SYNTHESIS:

Rearrangements in synthesis, photo chemistry in synthesis, pericyclic rearrangements in synthesis. Advanced strategy used in disconnection approach, Pro approach with typical examples for synthesis design.

Books:

(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) Frontier orbitals & organic chemical reactions by Ian Fleming. John Wiley & Sons(1978)
(4) Hand book of Heterocyclic Chemistry ,Alan R. Katritzky, Pergamon press(1985)
(5) Heterocyclic Chemistry by T.L. Gilchrist ,Pitman Publishing Ltd.(1985)
(6) Heterocyclic Chemistry by Joule & Smith, Van Norstand Reinhold (1989)
(7) Designing Organic synthesis: A programmed Introduction to Synthon Approach: Stuart Erren. John Wiley & Sons (1978)
(8) Organic Synthesis : The disconnection Approach. Stuart Warren. John Wiley & Sons (1982)
(9) The Logic Chemical synthesis by E.J Corey & X.M. Cheng. John Wiley & Sons (1989)
(10) Organic Synthesis Concepts, Methods & Starting Materials , Fuhrhop/Penzlin, VCH(1986)

(11) Organometallic Reagents in Synthesis (Oxford Chem.Primer).Paul R.jenkins. Oxford science publications
(12) Organic Synthesis : The role of Boron & Silicon (Oxford Chem. Primer) S.E. Thomas. Oxford science publication
(13) Organotransitional Metal chemistry: Application of Organic Synthesis.StephanG.Davies. Pergamon press(1982)
(14) Application of Functionalized Polymers in Organic Synthesis. Akelaah& D.C Sherrington.Chemical Reviews,81,557-587,198?
(15) Solid phase synthesis, Merrifield, Science, 232341-347,1986.
(16) Medicinal & Pharmaceutical Chemistry. Harkishansingh& V.K. Kapoor. VallabhPrakashan (1996).

CH 602 **ELECTIVE-I** **Full Marks: 50**

PHYSICAL CHEMISTRY-I

Objective: To understand phenomenon related to liquids, including theories of their structure and properties. The dynamic properties in solutions or during reactions are being also aimed at.

Outcome: The detail discussion during the course will help in understanding the concepts and properties of liquids/solutions.

UNIT-I

ATOMIC STRUCTURE:

Born-Oppenheimer Approximation, Hydrogen-Like Atoms, Helium-Like Atoms,

Hartree-Fock Scheme.

UNIT-II

EQUILIBRIUM THEORY OF LIQUIDS AND LIQUID MIXTURES:

Statistical Mechanics of Simple liquids, One dimensional fluids, Lattice gas and Lattice Models of liquid state.

UNIT-III

FAST IONIC REACTIONS:

Diffusion controlled Reactions between Ions in solution. Diffusion controller Ionic Reactions, Relaxation Experiments, Smoluchowski Equation, Debby modification. Flash photolysis, Electron transfer reaction.

Books

1. Quantum Chemistry — A. K Chandra
2. Quantum Chemistry — Donald D. Fitts
3. Quantum Chemistr — I. Levine
4. Statistical Mechanics — A. Maczek
5. Chemical Kinetics — Laidler

CH 602 **ELECTIVE-I** **Full Marks: 50**

INORGANIC CHEMISTRY-I

Objectives: To develop advanced concept on crystal field theory, inorganic reaction mechanism and photo chemistry

Outcome: The advance course will familiarize the student with recent development of chemical bonding in inorganic chemistry, different thermodynamic parameter on reaction mechanism and photo physical properties of different inorganic molecules.

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 d^2-system. The effect of weak octahedral field on S, P, D, and F, terms (quantitative). Correlation Diagram for d^2 system.

UNIT-II

LIGAND SUBSTITUTION REACTION:

Inorganic Nucleophilicity scales, nPt Scale, Methyl Hg(II) Scale. Edward Scale. Gutmann Donor Numbers, Hydrogen bonding scales, Drago E & C Scale, LFER regent charge effects, Solvent effects, Steric Effects, measures of ligand size cone angles, Activation volume (ΔV), Entropy of activation (ΔS), internal conjugate base mechanism, ligand substitution on labile transition metal ions Eigen Wilkins Mechanism, Substitution on Fe(III) and the proton ambiguity, kinetics of chelate formation and the chelate effect.

UNIT-III

INORGANIC PHOTOCHEMISTRY

Basic photochemical process.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.

Books recommended:

1. Inorganic Chemistry: W. W. Perterfield, Chapter-14(Addition Wesley Publishing Co.)
2. Rection Mechanism of Inorganic and organometallic Systems, R. B. Jordan(Ch. 7), (Oxford Press, N. Y. 1991)

CH 604 **ELECTIVE II** **Full Marks: 50**

ORGANIC CHEMISTRY-II

Objective:

To impart knowledge on synthetic methodology and use of organometallic compounds in organic synthesis.

Outcome:

1) Acquired knowledge on different methodology in organic synthesis

2) Understand the potential selectivity and reactivity of different organometallic reagents.
3) Understand the synthetic process of different drugs molecules.

UNIT-I

SYNTHETIC METHODOLOGY IN ORGANIC SYNTHESIS

Thedisconnection approach, Technical terms, Order of events,chemoselectivity,protecting groups,Regioselectivity,1,2,1,3,1,4,1,5,1,6 difunctionalised compounds,Radical reactions in synthesis,Reconnection strategy, strategy for ring synthesis, saturated heterocycles, rearrangements in synthesis, photo chemistry in synthesis, pericyclic rearrangements in synthesis. Advanced strategy used in the disconnection approach, Pro approach with typical examples for synthesis design.

UNIT- II

APPLICATION OF ORGANOMETALLICS IN ORGANIC SYNTHESIS

Use of Organometallic compounds of Mg,Li,Zn,Cd,Co,B,Si, organic synthesis. Rearrangements catalysed by metal ions and complexes.Catalysed synthetic processes including heterogeneous catalysts. A brief description of Phase transfer catalysis.Organic reactions and biocatalysts in Organic Synthesis.

UNIT-III

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.

CH 604 **ELECTIVE II** **Full Marks: 50**

PHYSICAL CHEMISTRY-II

Objective: To introduced to the concept of nanomaterials and its magnetic properties

Outcome: The in depth concept will help in pursing advance research in nanoscience.

PHYSICAL CHEMISTRY- II

Unit-I Properties of indivisual nanoparticles.

Metal nanoclusters: Magic numbers, Geometric structure, Electronic Structure, Bulk to nanotransition.

The Chemistry of nanostructures: Chemical Synthesis of nanostructure, Solgel Processing, Electrochemical Synthesis of nanostructures, Solution Synthesis, Reactivity of nanostructure.

Unit-II Bulk nanostructured material

Solid methods for preparation of disordered nanostructure, Methods of Synthesis, Metal nanoclusture composite glasses, Porous silicon.

Nanocomposites: Layered nanocomposites, nanowire composite composite of nanoparticles.

Nanostructured crystals: Natural nanocrystal, Tab-crystals of metal nano particles.

Unit-III Magnetism in nanostructures

Basis of Ferromagnetism: Behavior of powder of Ferromagnetic nanoparticles, Properties of single Ferromagnetic nanoparticles, Dynamics of individual magnetic nanoparticles, Measurements of super paramagnetism and the blocking temperature, nanopore containment of magnetic particles.

Ferrofluids, antiferromagnetic nanoparticles.

Bulk nanostructure magnetic material: Effect of nanosized grain structure on magnetic properties, Magnetoresistive material, Carbon nanostructured ferromagnets.

Books:

1. Nanostructured materials. Processing, properties and applications. Ed. Care C.Koch, Williums Andrew publishing, Norwich, USA.
2. An introduction to nanoscience and nanotechnology. Nouailhat, Wiley.
3. The Physics and Chemistry of nanosolids, F.J. Owners, C.P. Poole. Jr. and John Wiley.
4. Nanoscopic materials, Emil Roduner, RSC publishing, UK.

CH 604 **ELECTIVE II** **Full Marks: 50**

INORGANIC CHEMISTRY-II

Objective: To introduce the concept of reaction mechanism and bioinorganic chemistry.

Outcome: The course will develop the concept of important biological processes pertaining to different metals.

UNIT-I

MECHANISM OF REACTIONS OF COORDINATlON COMPOUNDS IN SOLUTIONS:
Mechanism of substitution reaction at the Cr(III), Pt(II) Centre in comparison with Co(III). 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-II

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.

UN IT-III

Biochemistry of nitrogen fixation: Mechanism of nitrogen fixation by nitrogenase, Model system studies on nitrogen fixation by coordination compounds.
Reactions of Carbonic anhydrase: Mechanism
Books.

1. Inorganic Chemistry of Biological Processes: by M.N. Hughos.
2. Inorganic Reaction Mechanism -Basolo and Pearson.
3. Advanced Inorganic Chemistry - Cotton and Wilkson.
4. Inorganic Reaction Mechanism - R.O. Wilkins

CH 606 **Dissertation** **Full marks 100**

Objective: Students will review articles in a particular topic

Outcome: Students will learn how to present a research topic

Students are required to submit a dissertation based on the work carried by him under the supervision of a faculty member before the theory examination for evaluation and the same is required to be presented.