DEPARTMENT OF CHEMISTRY ,OSMANIA UNIVERSTY
M.Sc.Chemistry I &II Semester (CBCS) Syllabus
(effective from academic year 2011-2012 for Campus and Constituent colleges excluding Affiliated and District PG Centers)
[UNDER RESTRUCTURED CBCS Scheme]
(Approved in the P.G. BOS meeting held on 08-9-2011 and 15-9-2012)

Semester I

	Hrs/week	Internal assessment	Semester exam	Total	Credits
CH101T	4	20 marks	80 marks	100 marks	4
CH102T	4	20 marks	80 marks	100 marks	4
CH103T	4	20 marks	80 marks	100 marks	4
CH104T	4	20 marks	80 marks	100 marks	4
CH151P (IC LAB)	6			75 marks	3
CH152P (OC LAB)	6			75 marks	3
CH153P (PC LAB)	6			75 marks	3
Total				**625 marks**	**25**

Semester II

	Hrs/week	Internal assessment	Semester exam	Total	Credits
CH201T	4	20 marks	80 marks	100 marks	4
CH202T	4	20 marks	80 marks	100 marks	4
CH203T	4	20 marks	80 marks	100 marks	4
CH204T	4	20 marks	80 marks	100 marks	4
CH251P (IC LAB)	6			75 marks	3
CH252P (OC LAB)	6			75 marks	3
CH253P (PC LAB)	6			75 marks	3
Total				**625 marks**	**25**

Semester-I and Semester-II syllabus is common for all specializations i.e., Inorganic, Analytical, Organic, Physical, Pharmacoinformatics and Physical-Organic.and Pharmaceutical chemistry

DEPARTMENT OF CHEMISTRY
OSMANIA UNIVERSITY
(effective from academic year 2009-2010 for Campus and Constituent colleges excluding District PG Centers)
[UNDER CBCS Scheme]

Semester 1

	Hrs/week	Internal assessment	Semester exam	Total	Credits	
CH101T (*)	4	20 marks	80 marks	100 marks		4
CH102T (*)	4	20 marks	80 marks	100 marks		4
CH103T (*)	4	20 marks	80 marks	100 marks		4
CH104T (*)	4	20 marks	80 marks	100 marks		4
CH151P (IC LAB*)	6			75 marks		3
CH152P (OC LAB*)	6			75 marks		3
CH153P (PC LAB*)	6			75 marks		3
Total				**625 marks**		**25**

(*Core= compulsory papers common to all students admitted to M.ScChemistry,OU)

Semester 2

	Hrs/week	Internal assessment	Semester exam	Total	Credits	
CH201T (*)	4	20 marks	80 marks	100 marks		4
CH202T (*)	4	20 marks	80 marks	100 marks		4
CH203T (*)	4	20 marks	80 marks	100 marks		4
CH204T (*)	4	20 marks	80 marks	100 marks		4
CH251P (IC LAB*)	6			75 marks		3
CH252P (OC LAB*)	6			75 marks		3
CH253P (PC LAB*)	6			75 marks		3
Total				**625**	**marks**	**25**

(*= compulsory papers common to all students admitted to M.ScChemistry,OU)

M.Sc CHEMISTRY SYLLABUS

(Effective from academic year 2009-2010 for Campus and Constituent colleges
excluding Affiliated and District PG Centers
***And from 2012-2012 for University College for Women for Pharmaceutical Chemistry*)**

SEMESTER –I

Semester-I and Semester-II syllabus is common for all specializations i.e., Inorganic-Analytical, Organic, Physical, Chemistry-Pharmacoinformatics and Physical- Organic. and Pharmaceutical Chemistry)

THEORY PAPERS
PAPER I: CH(IC) 101T (INORGANIC CHEMISTRY)
PAPER II: CH(OC) 102 T(ORGANIC CHEMISTRY)
PAPER III:CH(PC) 103T (PHYSICAL CHEMISTRY)
PAPER IV: CH (ATS)104T ANALYTICAL TECHNIQUES and SPECTROSCOPY

LABORATORY COURSE
PAPER V: CH (IC)151P: Inorganic chemistry LabCourse
PAPER VI: CH(OC) 152P: Organic Chemistry Lab course
PAPER VII: CH(PC) 153P: Physical Chemistry Lab course

SEMESTER –II

(Semester-I and Semester-II syllabus is common for all specializations i.e., Inorganic-Analytical, Organic, Physical, Chemistry-Pharmacoinformatics and Physical-Organic. and Pharmaceutical Chemistry)

PAPER I: CH(IC) 201T: INORGANIC CHEMISTRY
PAPERII:CH(OC) 202 T: ORGANIC CHEMISTRY
PAPERIII:CH(PC) 203T: PHYSICAL CHEMISTRY
PAPER IV: CH(ATS) 204T:ANALYTICAL TECHNIQUES and SPECTROSCOPY

PAPERV:CH(IC) 251P : Inorganic chemistry Lab
PAPER VI: CH (OC)252P Organic Chemistry Lab
PAPER VII:CH (PC)253P :Physical Chemistry Lab

PAPER TITLES

M.Sc. INORGANIC CHEMISTRY SPECIALISATION

III SEMESTER SYLLABUS

(For the batch admitted during the academic year 2011-2012 under the CBCS pattern)

[Under Restructured CBCS Scheme]

THEORY PAPERS

PAPER-1 CH(IC)301T: Bonding, Group Theory and its Applications

IC-09: Group Theory, Normal mode analysis and Spectral Activity

IC-10: MOT of Metal Complexes

IC-11: Electronic Spectroscopy of Metal Complexes

IC-12: IR and Raman Spectroscopy

PAPER-II CH(IC) 302T : Molecular Spectroscopy of Inorganic Compounds

IC-13: Multinuclear NMR

IC-14: Advanced NMR techniques

IC-15 Applications of ESR to Metal Complexes

IC-16 : Mossbauer Specroscopy and Nuclear Quadrupole Resonance Spectroscopy

PAPER-III CH(IC)303T : Organo metallic Chemistry of Transition Metal Complexes

IC-17: Mono,Di and Tri hapto Complexes

IC-18: Tetra,Penta,Hexa,Hepta and Octahapto Complexes

IC-19: Catalytic Role of OTMC-I

IC-20: Catalytic Role of OTMC-II

PAPER-IVCH(IC) 304T : Photochemistry, Thermal , Diffraction and Mass spectrometry Methods

IC-21: Photochemistry of Metal Complexes

IC-22: Thermal Methods, AAS, AES, ICP-AES

IC-23:, Diffraction Methods

IC-24: Advanced Mass spectrometry & Hyphenated Techniques

LABORATORY COURSES

PAPER-V CH (IC) 351P: Synthesis and Characterization of Metal Complexes

PAPER–VI CH (IC) 352 P: Electro-analytical techniques

PAPER TITLES

M.Sc. INORGANIC CHEMISTRY SPECIALISATION

IV SEMESTER SYLLABUS

(For the batch admitted during the academic year 2011-2012 under the CBCS pattern)

[Under Restructured CBCS Scheme]

THEORY PAPERS

PAPER-I CH(IC) 40T1: Inorganic Biochemistry

IC-25: Metal ions Interactions with Nucleic acids and their constituents.
IC-26: Transport of Electrons and Metal ions.
IC-27: Metallo-Enzymes of Iron,Zinc and Nickel.
IC-28: Metallo-Enzymes of Cobalt,Copper and Molybdenum.

PAPER-II CH (IC) 402T: Medicinal Inorganic Chemistry

IC-29: Metal complexes as Drugs and Anticancer agents
IC-30: Metal complexes in Clinical Chemistry
IC-31: Chemical and Photochemical probing of DNA complexes
IC-32: DNA binding and molecular pharmacology and Interaction of Metallo Pharmaceuticals

PAPER-III CH(IC) 403T: Supra Molecular Chemistry and Bio Physical Studies

IC-33: Supramolecular Chemistry
IC-34: Structural aspects of DNA and RNA
IC-35: Spectroscopic analysis of drug/metal complexes binding to Nucleic acid:
IC-36: CD ,ORD, Fluorescence and Enzyme kinetics

PAPER-IV CH(IC) 404T(CB_1): Separation Methods, Data Handling, Green Chemistry and Nanotechnology

IC (CB_1)-1: Separation Methods
IC (CB_1)-2: Data Handling
IC (CB_1)-3: Green Chemistry
IC (CB_1)-4: Nanotechnology

PAPER-IV CH(IC) 404T (CB_2) : Applied Analysis

IC (CB_2)-1: Data Handling
IC (CB_2)-2: Analysis of Air and Water Pollutants
IC (CB_2)-3: Clinical and Pharmaceutical analysis
IC (CB_2)-4: Food and Agricultural analysis

LABORATORY COURSES

PAPERV CH (IC) 451P: Spectroscopic techniques

PAPERVI CH (IC) 452P: Structural Assignment of Metal Complexes from Physico-Chemical Data &ConventionaLMethods of Analysis

PAPER TITLES

M.Sc. ORGANIC CHEMISTRY SPECIALISATION

III SEMESTER SYLLABUS

(For the batch admitted during the academic year 2011-2012 under the CBCS pattern)

[Under Restructured CBCS Scheme]

THEORY PAPERS

PAPER-1CH(OC) 301T: Conformational Analysis, Asymmetric Synthesis and Biomolecules

OC09: Conformational Analysis (cyclic systems)

OC10: Principles of Asymmetric synthesis

OC11: Methodologies in asymmetric synthesis

OC12: Biomolecules

PAPER-II– CH (OC) 302T: Modern Organic Synthesis

OC13- Synthetic Reagents I

OC 14- Synthetic Reagents II

OC 15- New Synthetic reactions

OC 16- New techniques and concepts in organic synthesis

PAPER-III: CH (OC) 303T: Organic Spectroscopy and Pericyclic reactions.

OC-17: ^{13}C NMR spectroscopy

OC-18: 2D NMR techniques and ORD

OC-19: Pericyclic reactions I

OC-20: Pericyclic reactions II

PAPER-IV CH (OC) 304T: Photochemistry, synthetic strategies and Green Chemistry

OC-21 Photochemistry

OC-22 Synthetic strategies - I

OC-23 Synthetic strategies - II

OC-24 Green Chemistry

LABORATORY COURSES

PAPER-V CH (O) 351P: Separation and identification of organic compounds

PAPER VICH (O)352P: Synthesis of organic molecules & isolation of natural products

PAPER TITLES

M.Sc. ORGANIC CHEMISTRY SPECIALISATION

IV SEMESTER SYLLABUS

(For the batch admitted during the academic year 2011-2012 under the CBCS pattern)

[Under Restructured CBCS Scheme]

THEORY PAPERS

PAPER-1 CH (OC) 401T: Drug Design and Drug Discovery

OC-25: Principles of Drug design and drug discovery

OC-26: Lead modification and SAR Studies

OC 27: QSAR studies

OC 28: Combinatorial Synthesis

PAPER-II CH (OC) 402T: Drug synthesis and mechanism of action

OC-29: Drugs acting on metabolic process, cell wall and specific enzymes

OC-30: Drugs acting on genetic material and immune system

OC-31: Drugs acting on receptors and ion channels

OC-32: Chiral drugs

PAPER-III CH (OC) 403T: Advanced Heterocyclic Chemistry

OC-33: Non aromatic heterocyclics

OC-34: Five and six membered heterocyclics with two hetero atoms

OC-35: Heterocyclics with more than two hetero atoms

OC-36: Larger ring and other heterocycles

PAPER-IV CH (OC) 404T(CB_1): Advanced Natural Products

OC(CB_1)-1: Biosynthesis of natural products

OC(CB_1)-2-: Structure determination and stereochemistry of natural products by chemical methods.

OC(CB_1)—3: Structure determination and stereochemistry of natural products by spectral methods.

OC(CB_1)—4: Total stereo selective synthesis of natural products.

PAPER-IV CH (OC) 404T (CB_2): Bioorganic Chemistry

OC (CB_2) -1: Enzymes and their action

OC (CB_2) -2: Enzyme models and Enzymatic transformations

OC (CB_2) -3: Recombinant DNA and Fermentation technology

OC (CB_2) -4: Coenzymes

PAPER-IV CH (OC) 404T (CB_3): Physical- Organic Chemistry

OC (CB_3) -1: MO and VB theory of reactivity

OC (CB_3) -2: Kinetic, isotopic, structural, solvent, steric and conformational effects

OC (CB_3) -3: Nucleophilic, electrophilic and free radical reactivity

OC (CB_3) -4: Supramolecular chemistry

Laboratory courses

PAPER-V CH(OC) 451P: Spectroscopic identification of organic compounds and Chromatography.

PAPER-VI CH(OC) 452P: Synthesis and analysis of drugs

PAPER TITLES

M.Sc. PHYSICAL CHEMISTRY SPECIALISATION

III SEMESTER SYLLABUS

(For the batch admitted during the academic year 2011-2012 under the CBCS pattern)

[Under Restructured CBCS Scheme]

THEORY PAPERS

PAPER-I CH(P) 301T: Chemical Kinetics, Photochemistry Electrochemistry&Supramolecularchemistry

PC-09 : Chemical Kinetics-II

PC-10 : Photochemistry-II

PC-11 : Electrochemistry -II

PC-12 : Supramolecular Chemistry

PAPER-II CH (P) 302T : Spectroscopy & Lasers

PC- 13: Physical principles of spectroscopy & Vibrational spectroscopy

PC- 14: NMR , NQR and Mossbaur Spectroscopy

PC- 15: X-ray Spectroscopy & Diffraction techniques

PC- 16: lasers in Chemistry

PAPER-III CH(P) 303T: Quantumchemistry and Group Theory

PC –17: Applications of Schrödinger equation

PC - 18: Angular momentum & approximate methods

PC - 19: Bonding in molecules

PC - 20: Group theory

PAPER-IV CH(P) 304: Polymer Chemistry

PC- 21: Polymerization & Kinetics of polymerization

PC- 22: Structure and properties of polymers

PC- 23: Processing of Polymers

PC- 24: Functional polymers

LABORATORY COURSES

PAPER-V CH(P) 351P:Chemical Kinetics

PAPER-VI CH(P) 352P: Instrumentation

PAPER TITLES

M.Sc. PHYSICAL CHEMISTRY SPECIALISATION

IV SEMESTER SYLLABUS

(For the batch admitted during the academic year 2011-2012 under the CBCS pattern)

[Under Restructured CBCS Scheme]

THEORY PAPERS

PAPER-1 CH(P) 401: Thermodynamics& ComputationalChemistry.

PC-25 : Statistical Thermodynamics

PC-26 : Non-equilibrium Thermodynamics

PC-27 : Computational Chemistry

PC-28 : Theoretical treatment of bio polymers

PAPER-2 CH(P)402 :Applied Chemistry and Material Science

PC-30 : Applied Electrochemistry

PC-31 : Types of materials, conducting organics and NLO materials

PC-29 : Applied kinetics

PC-32 : Liquid crystals and nanoparticles

PAPER-3 CH(P) 403 : Catalysis

PC- 33: Homogeneous catalysis

PC-34: Surface Chemistry &Micellar catalysis

PC-35: Heterogeneous catalysis

PC-36: Phase transfer , Anchored & Photo catalysis

PAPER-4 CH(P) 404T(CB_1): Engineering Chemistry

PC(CB_1) -1: Water and waste water treatment

PC(CB_1) -2: Corrosion and its control

PC(CB_1) -3: Energy sources:

PC(CB_1)- 4: Engineering materials.

PAPER-4CH(P) –404T(CB_2) : Computational Chemistry&It's Applications

PC(CB_2)-1: Computational Chemistry – I

PC(CB2)-2: Computational Chemistry – I

PC(CB_2)-3: Drug Design Methods I - Ligand Based

PC(CB_2)-4: Drug Design Methods II - Structure Based.

LABORATORY COURSES

PAPER-V CH(P) 451P:Chemical Kinetics

PAPER-VI CH (P) 452P:Instrumentatio

PAPER TITLES

M.Sc. PHYSICAL ORGANIC CHEMISTRY SPECIALISATION

IV SEMESTER SYLLABUS

(For the batch admitted during the academic year 2011-2012 under the CBCS pattern)

[Under Restructured CBCS Scheme]

THEORY PAPERS

PAPER-1CH(PO) 301T:Chemical Kinetics, Catalysis and Electrochemistry

PO- 09: Chemical Kinetics-II
PO- 10: Heterogeneous, Phase-transfer& Enzyme catalysis
PO- 11: Polymerization & Kinetics of polymerization
PO- 12: Electrochemistry-II

PAPER-II CH(PO)302T:Thermodynamics,Supramolecular Chemistry and Nanoparticles

PO- 13:Statistical Thermodynamics
PO- 14: Non equilibrium Thermodynamics
PO- 15: Supramolecular Chemistry
PO- 16: Nanoparticles

PAPER-III CH(PO)303T: Conformational Analysis, Asymmetric synthesis and Synthetic strategies

PO- 17: Conformational Analysis (Cyclic Systems)
PO- 18: Principles of Asymmetric synthesis
PO- 19: Methodology of asymmetric synthesis
PO- 20: Synthetic strategies

PAPER-IV CH(PO) 304T: Modern Organic Synthesis

PO- 21: Synthetic Reagents I
PO- 22: Synthetic Reagents II
PO- 23: New synthetic reactions
PO- 24: New techniques and concepts in organic synthesis

LABORATORY COURSES

CH(PO) 351P: Chemical Kinetics (Paper-V)

CH(PO) 352P:Organic Synthesis and chromatography(Paper-VI)

PAPER TITLES

M.Sc. PHYSICAL ORGANIC CHEMISTRY SPECIALIZATION

IV SEMESTER SYLLABUS

(For the batch admitted during the academic year 2011-2012 under the CBCS pattern)

[Under Restructured CBCS Scheme]

THEORY PAPERS

PAPER-I-CH(PO) 401T: Spectroscopy , photochemistry and lasers in chemistry

PO- 25 : Physical principles of spectroscopy & Vibrational spectroscopy

PO- 26 : X-Ray Spectroscopy & Diffraction techniques

PO- 27: Photochemistry – II

PO- 28: Lasers in chemistry

PAPER- II- CH(PO) 402T: Quantum Chemistry and Group Theory

PO- 29: Applications of Schrödinger equation

PO- 30: Angular momentum & approximate methods

PO- 31: Bonding in molecules

PO- 32: Group Theory

PAPER- III: CH (PO) 403T: Organic Spectroscopy and Pericyclic Reactions.

PO-33: ^{13}C NMR spectroscopy

PO-34: 2D NMR techniques and ORD

PO-35: Pericyclic reactions I

PO-36: Pericyclic reactions II

PAPER-IV CH(PO) 404T(CB_1):Heterocyclics ,Biomolecules, Green Chemistry , Principles of drug design &Discovery

PO-(CB_1)- 1: Five and six membered heterocyclics with two hetero atoms

PO-(CB_1)- 2: Biomolecules

PO-(CB_1) - 3: Green chemistry

PO-(CB_1) - 4: Principles of drug design and discovery

PAPER-IVCH (PO) 404T(CB_2): Modern material Chemistry & Combinatorial Chemistry

PO-(CB_2)-1: Types of materials, Conducting Organics and NLO materials

PO-(CB_2)-2: Functional Polymers

PO-(CB_2)-3: Dynamics of biopolymers

PO-(CB_2)-4: Combinatorial Chemistry

PAPER-IV CH (PO) 404T(CB_3):Biopolymer chemistry

PO-(CB_3)- 1: Bioenergetics & physical properties of biopolymers

PO-(CB_3)-2: Biological membranes & binding of ligands by biopolymers

PO-(CB_3) -3: DNA, genes & cloning

PO-(CB_3) -4: Bioinformatics

LABORATORY COURSES

PAPER – VCH(PO) 451P: Instrumentation

PAPER-VI CH(PO) 452P : Separation , Identification of Organic compounds and spectral analysis

PAPER TITLES

M.Sc. PHARMACOINFORMATICS SPECIALIZATION

IV SEMESTER SYLLABUS

(For the batch admitted during the academic year 2011-2012 under the CBCS pattern)

[Under Restructured CBCS Scheme]

SEMESTER – III

PAPER- I CH(CPI)301 T : Database Management, Sources and Scripting Languages

CPI - 09 : Chemical Information Sources and Searches
CPI - 10 : Database Design and Management
CPI - 11 : Data Sequencing and Mining
CPI - 12 : Scripting Languages

PAPER-II CH(CPI)302T: Principles of DrugDiscovery,Development and Drug Targets

CPI - 13 : Principles of Drug Discovery
CPI - 14 : SAR Studies
CPI - 15 : Combinatorial Synthesis
CPI - 16 : General Principles of Pharmacology and drug Targets

PAPER-III CH(CPI)303 T :Chemistry of Pharmacology

CPI - 17 : Pharmacology of Drugs Acting on ANS and CNS
CPI - 18 : Drugs Acting on Cardio Vascular & Respiratory System
CPI - 19 : Drugs acting on metabolic process and cell wall
CPI - 20 : Drugs acting on genetic material and immune system

PAPER-IV CH(CPI)304 T:Computational Chemistry ,Molecular Modeling &Its Applications.

CPI – 21 : Computational Chemistry I
CPI – 22 : Computational Chemistry II
CPI – 23: Drug Design Methods I - Ligand Based
CPI – 24 : Drug Design Methods II – Structure Based

LABORATORY COURSES

PAPER-V CH(CPI)351 P : Molecular Modelling Lab

PAPER-VI CH(CPI)352 P:Synthesis,Characterisation ofPharmaceuticals -Chromatographicand Spectral Techniques

PAPER TITLES

M.Sc. PHARMACOINFORMATICS SPECIALIZATION

IV SEMESTER SYLLABUS

(For the batch admitted during the academic year 2011-2012 under the CBCS pattern)

[Under Restructured CBCS Scheme]

SEMESTER – IV

PAPER–ICH(CPI)401T : Strategies in Drug Synthesis (SDS)

CPI - 25 : Nitrogen Heterocycles& nucleic acids
CPI - 26 : Synthetic strategies
CPI - 27: Stereoselective Synthesis
CPI - 28 : Chiral Drug

PAPER- II CH(CPI) 402T : Pharmaceutical Analysis

CPI - 29: Spectral Methods in Pharmaceutical Analysis
CPI - 30: Chromatography in Pharmaceutical Analysis-I
CPI -31:Chromatography in Pharmaceutical Analysis-II
CPI - 32: Titrimetry, Chemical and Extraction methods in Pharmaceutical Analysis

PAPER– III CH(CPI) 403 T Pharmacokinetics

CPI - 33 : Biopharmaceutics
CPI - 34 :Drug AbsorptionandDistribution
CPI - 35 : Drug MetabolismandExcretion
CPI - 36 : Pharmacokinetic Models

PAPER-IV CH(CPI) 404T ($CB_{1)}$:Intellectual Property Rights

CPI(CB_1)-1 : - : Introduction
CPI(CB_1)-2: - 30: International Organizations & Treaties
CPI (CB_1)-3: Patent Search
CPI (CB_1)-4: IP Reports Generation

PAPER-IV CH(CPI) 404T (CB_2) :Organic Synthesis , Pericyclic Reactions and Photochemistry

CPI(CB_1)-1: Synthetic Reagents :(Oxidations, Reductions and organometallic reagents)
CPI (CB_2)-2: Newsynthetic reactions
CPI (CB_3): Pericyclic Reactions
CPI (CB_4): Photochemistry

LABORATORY COURSES

PAPER–V CH(CPI)451 P: Quantitative Analysis of Pharmaceuticals

PAPER – VI CH(CPI) 452: Project Work

PAPER TITLES

M.Sc. ANALYTICAL CHEMISTRY SPECIALIZATION

IV SEMESTER SYLLABUS

(For the batch admitted during the academic year 2011-2012 under the CBCS pattern)

[Under Restructured CBCS Scheme]

SEMESTER-III

PAPER-I:CH(AC)301T: Sampling, Data handling, Classical and Atomic Spectral methods of analysis

AC – 09 Sampling & Data handling
AC – 10 Titrimetric & Gravimetric analysis
AC – 11 Thermal & Radiochemical methods of analysis
AC – 12Atomic Spectroscopy

PAPER-II:CH(AC)302T: Spectroscopic methods of Analysis-I

AC – 13 Multinuclear NMR
AC – 14 Advanced NMR
AC – 15 Electron Spin Resonance Spectroscopy
AC – 16Mossbauer and NQR

PAPER-III:CH(AC)303T: Spectroscopic methods of Analysis-II

AC – 17 U.V. visible spectroscopy,
AC –18 IR & Raman spectroscopy
AC – 19 Optical Methods
AC – 20Fluorimetry, Phosphorimetry,Nephelometry and Turidimetry

PAPER-IV:CH(AC)304T: Separation Methods

AC- 21 Solvent extractions
AC –22 Chromatography
AC –23 Mass spectrometry & Hyphenated techniques
AC –24 Electrophoresis

LABORATORY COURSE

PAPER –V CH(AC)351P: Titrimetry, Solvent extraction,Chromatography and Water analysis.

Paper CH (AC) 352P: Colorimetry, Spectrophotometry

PAPER TITLES

M.Sc. ANALYTICAL CHEMISTRY SPECIALIZATION

IV SEMESTER SYLLABUS

(For the batch admitted during the academic year 2011-2012 under the CBCS pattern)

[Under Restructured CBCS Scheme]

SEMESTER-IV

PAPER-I CH (AC) 401T: Miscellaneous Methods of Analysis

AC - 25 Surface Analysis Methods
AC –26 Diffraction Methods, X-Ray Absorption and X-Ray Fluorescence
AC –27 Electroanalytical Methods
AC –28 Micromeritics, Dissolution and disintegration

PAPER-II CH(AC) 402T:Applied Analysis

AC –29 Industrial Analysis
AC –30Analysis of Air and Water Pollutants
AC – 31 Clinical and Pharmaceutical analysis
AC – 32 Food and Agricultural analysis

PAPER-III CH(AC)403T: Laboratory Management

AC – 33 Automation in laboratory
AC – 34 LIMS & Computer aided analysis
AC – 35 Laboratory Management & Standard reference materials
AC – 36 Accreditation of Laboratories, Quality management

PAPER-IV: CH (AC)404T(CB_1) : Quality Assurance and Accreditation

AC(CB_1) -1 Quality Assurance – I
AC(CB_1) -2 Quality Assurance – II
AC(CB_1) -3 Quality Assurance – III
AC(CB_1)- 4 Quality Accreditation

PAPER – IV: CH (AC)404T(CB_2) : Applied analysis and Green Analytical Chemistry

AC(CB_2) -1 Enzyme catalysis- Analytical applications
AC(CB_2) -2 Forensic Chemical Analysis
AC(CB_2) -3 Limit tests
AC(CB_2)- 4 Green Analytical Chemistry

LABORATORY COURSE

PAPER- V CH (AC) 451P: Electro Analytical Techniques:

PAPER-VI CH(AC) 452P: Spectroscopy and Evaluation of Physical Parameters of Tablets

PAPER TITLES(2012-2013)

M.Sc. INORGANIC CHEMISTRY SPECIALISATION

III SEMESTER SYLLABUS

(For the batch admitted during the academic year 2011-2012 under the CBCS pattern)

[Under Restructured CBCS Scheme]

SEMESTER-III

THEORY PAPERS

PAPER-1: CH(IC)301T: Bonding, Group Theory and its Applications

PAPER-II :CH(IC) 302T : Molecular Spectroscopy of Inorganic Compounds

PAPER-III: CH(IC)303T : Organo metallic Chemistry of Transition Metal Complexes

PAPER-IV:CH(IC) 304T :Photochemistry, Thermal , Diffraction and Mass spectrometry Methods

LABORATORY COURSES

PAPER-V : CH (IC) 351P: Synthesis and Characterization of Metal Complexes

PAPER–VI :CH (IC) 352 P: Electro-analytical techniques

PAPER TITLES

M.Sc. INORGANIC CHEMISTRY SPECIALISATION

IV SEMESTER SYLLABUS

(For the batch admitted during the academic year 2011-2012 under the CBCS pattern)

[Under Restructured CBCS Scheme]

SEMESTER-IV

THEORY PAPERS

PAPER-I: CH(IC) 40T1: Inorganic Biochemistry

PAPER-II: CH (IC) 402T: Medicinal Inorganic Chemistry

PAPER-III: CH(IC) 403T: Supra Molecular Chemistry and Bio Physical Studies

PAPER-IV: CH(IC) 404T(CB_1): Separation Methods, Data Handling, Green Chemistry and Nanotechnology

PAPER-IV :CH(IC) 404T (CB_2) : Applied Analysis

LABORATORY COURSES

PAPER V:CH (IC)451P: Spectroscopic techniques

PAPER VI :CH (IC)452P: Structural Assignment of Metal Complexes from Physico-Chemical Data &Conventional Methods of Analysis

PAPER TITLES(2012-2013)

M.Sc. ORGANIC CHEMISTRY SPECIALISATION

III SEMESTER SYLLABUS

(For the batch admitted during the academic year 2011-2012 under the CBCS pattern)

[Under Restructured CBCS Scheme]

SEMESTER-III

THEORY PAPERS

PAPER-1:CH(OC) 301T: Conformational Analysis, Asymmetric Synthesis and Biomolecules

PAPER-II:CH (OC) 302T: Modern Organic Synthesis

PAPER-III:CH(OC) 303T:Organic Spectroscopy and Pericyclic reactions.

PAPER-IV: CH(OC)304T:Photochemistry, synthetic strategies and Green Chemistry

LABORATORY COURSES

PAPER-V :CH (O) 351P: Separation and identification of organic compounds

PAPER VI:CH (O)352P: Synthesis of organic molecules & isolation of natural products

PAPER TITLES(2012-2013)

M.Sc. ORGANIC CHEMISTRY SPECIALISATION

IV SEMESTER SYLLABUS

(For the batch admitted during the academic year 2011-2012 under the CBCS pattern)

[Under Restructured CBCS Scheme]

SEMESTER-IV

THEORY PAPERS

PAPER-1: CH (OC) 401T: Drug Design and Drug Discovery

PAPER-II :CH (OC) 402T: Drug synthesis and mechanism of action

PAPER-III:CH (OC) 403T: Advanced Heterocyclic Chemistry

PAPER-IV:CH (OC) 404T(CB_1): Advanced Natural Products

PAPER-IV: CH (OC) 404T (CB_2): Bioorganic Chemistry

PAPER-IV:CH (OC) 404T (CB_3): Physical- Organic Chemistry

LABORATORY COURSE

PAPER-V:CH(OC) 451P: Spectroscopic identification of organic compounds and Chromatography:

PAPER-VI: CH(OC) 452P: Synthesis and analysis of drugs

PAPER TITLES(2012-2013)

M.Sc. PHYSICAL CHEMISTRY SPECIALISATION

III SEMESTER SYLLABUS

(For the batch admitted during the academic year 2011-2012 under the CBCS pattern)

[Under Restructured CBCS Scheme]

SEMESTER-III

THEORY PAPERS

PAPER-I: CH(P) 301T: Chemical Kinetics, Photochemistry Electrochemistry&Supramolecularchemistry

PAPER-II:CH (P) 302T : Spectroscopy & Lasers

PAPER-III:CH(P) 303T: Quantumchemistry and Group Theory

PAPER-IV: CH(P) 304: Polymer Chemistry

LABORATORY COURSES

PAPER-V :CH(P) 351P:Chemical Kinetics

PAPER-VI :CH(P) 352P: Instrumentation

PAPER TITLES(2012-2013)

M.Sc. PHYSICAL CHEMISTRY SPECIALISATION

IV SEMESTER SYLLABUS

(For the batch admitted during the academic year 2011-2012 under the CBCS pattern)

[Under Restructured CBCS Scheme]

SEMESTER-IV

THEORY PAPERS

PAPER-I:CH(P) 401: Thermodynamics& ComputationalChemistry.

PAPER-II:CH(P)402 :Applied Chemistry and Material Science

PAPER-III: CH(P) 403 : Catalysis

PAPER-IV:CH(P) 404(CB_I): Engineering Chemistry

PAPER-IV:CH(P)404(CB_2) : Computational Chemistry&It's Applications

LABORATORY COURSES

PAPER-V :CH(P) 451P:Chemical Kinetics

PAPER-VI :CH (P) 452P: Instrumentation

PAPER TITLES(2012-2013)

M.Sc. PHYSICAL ORGANIC CHEMISTRY SPECIALISATION

IV SEMESTER SYLLABUS

(For the batch admitted during the academic year 2011-2012 under the CBCS pattern)

[Under Restructured CBCS Scheme]

SEMESTER-III

THEORY PAPERS

PAPER-1:CH(PO) 301T:Chemical Kinetics, Catalysis and Electrochemistry

PAPER-II :CH(PO)302T:Thermodynamics,Supramolecular Chemistry and Nanoparticles

PAPER-III:CH(PO)303T: Conformational Analysis , Asymmetric synthesis and Synthetic strategies

PAPER-IV:CH(PO) 304T: Modern Organic Synthesis

LABORATORY COURSES

PAPER-V: CH(PO) 351P: Chemical Kinetics

PAPER-VI:CH(PO) 352P:Organic Synthesis and chromatography

PAPER TITLES(2012-2013)

M.Sc. PHYSICAL ORGANIC CHEMISTRY SPECIALIZATION

IV SEMESTER SYLLABUS

(For the batch admitted during the academic year 2011-2012 under the CBCS pattern)

[Under Restructured CBCS Scheme]

THEORY PAPERS

PAPER-I:CH(PO) 401T: Spectroscopy , photochemistry and lasers in chemistry

PAPER- II: CH(PO) 402T: Quantum Chemistry and Group Theory

PAPER- III: CH (PO) 403T: Organic Spectroscopy and Pericyclic Reactions.

PAPER-IV: CH(PO) 404T(CB_1):Heterocyclics ,Biomolecules, Green Chemistry , Principles of drug design &Discovery

PAPER-IV:CH (PO) 404T(CB_2): Modern material Chemistry & Combinatorial Chemistry

PAPER-IV:CH (PO) 404(CB_3)T:Biopolymer chemistry

LABORATORY COURSES

PAPER – V :CH(PO) 451P: Instrumentation

PAPER- VI :CH(PO) 452P : Separation & Identification of Organic compounds and spectral analysis

PAPER TITLES(2012-2013)

M.Sc. CHEMISTRY-PHARMACOINFORMATICS SPECIALIZATION

IV SEMESTER SYLLABUS

(For the batch admitted during the academic year 2011-2012 under the CBCS pattern)

[Under Restructured CBCS Scheme]

SEMESTER – III

THEORY PAPERS

PAPER- I: CH(CPI)301 T : Database Management, Sources and Scripting Languages

PAPER-II: CH(CPI)302T: Principles of Drug Discovery,Development and Drug Targets

PAPER-III:CH(CPI)303 T :Chemistry of Pharmacology

PAPER-IV:CH(CPI)304 T:Computational Chemistry ,Molecular Modeling &Its Applications.

LABORATORY COURSES

PAPER-V :CH(CPI)351 P : Molecular Modelling Lab

PAPER-VI: CH (CPI)352 P:Synthesis,Characterisation ofPharmaceuticals - Chromatographic and Spectral Techniques

PAPER TITLES(2012-2013)

M.Sc. PHARMACOINFORMATICS SPECIALIZATION

IV SEMESTER SYLLABUS

(For the batch admitted during the academic year 2011-2012 under the CBCS pattern)

[Under Restructured CBCS Scheme]

SEMESTER – IV

PAPER –I:CH(CPI)401T : Strategies in Drug Synthesis (SDS)

PAPER- II :CH(CPI) 402T : Pharmaceutical Analysis

PAPER – III :CH(CPI) 403:T Pharmacokinetics

PAPER-IV :CH(CPI) 404T ($CB_{1)}$:Intellectual Property Rights

PAPER-IV: CH(CPI) 404T (CB_2) :Organic Synthesis , Pericyclic Reactions and Photochemistry

LABORATORY COURSES

PAPER–V :CH(CPI)451 P: Quantitative Analysis of Pharmaceuticals

PAPER – VI: CH(CPI) 452: Project Work

PAPER TITLES(2012-2013)

M.Sc. ANALYTICAL CHEMISTRY SPECIALIZATION

IV SEMESTER SYLLABUS

(For the batch admitted during the academic year 2011-2012 under the CBCS pattern)

[Under Restructured CBCS Scheme]

SEMESTER-III

THEORY PAPERS

PAPER-I:CH(AC)301T: Sampling, Data handling, Classical and Atomic

PAPER-II:CH(AC)302T: Spectroscopic methods of Analysis-I

PAPER-III:CH(AC)303T: Spectroscopic methods of Analysis-II

PAPER-IV:CH(AC)304T: Separation Methods

LABORATORY COURSE

PAPER –V: CH(AC)351P: Titrimetry, Solvent extraction,Chromatography and Water analysis.

PAPER-VI:CH (AC) 352P: Colorimetry, Spectrophotometry

PAPER TITLES

M.Sc. ANALYTICAL CHEMISTRY SPECIALIZATION

IV SEMESTER SYLLABUS

(For the batch admitted during the academic year 2011-2012 under the CBCS pattern)

[Under Restructured CBCS Scheme]

SEMESTER-IV

PAPER-I :CH (AC) 401T: Miscellaneous Methods of Analysis

PAPER-II :CH(AC) 402T:Applied Analysis

PAPER-III :CH(AC)403T: Laboratory Management

PAPER-IV: CH (AC)404T(CB_1) : Quality Assurance and Accreditation

PAPER – IV: CH (AC)404T(CB_2) : Applied analysis and Green Analytical Chemistry

LABORATORY COURSE

PAPER- V:CH (AC) 451P: Electro Analytical Techniques:

PAPER-VI :CH(AC) 452P: Spectroscopy and Evaluation of Physical Parameters of Tablets

DEPARTMENT OF CHEMISTRY
OSMANIA UNIVERSITY
(effective from academic year 2009-2010 for Campus and Constituent colleges excluding District PG Centers)
[UNDER CBCS Scheme]

Semester 1

	Hrs/week	Internal assessment	Semester exam	Total	Credits
CH101T (*)	4	20 marks	80 marks	100 marks	4
CH102T (*)	4	20 marks	80 marks	100 marks	4
CH103T (*)	4	20 marks	80 marks	100 marks	4
CH104T (*)	4	20 marks	80 marks	100 marks	4
CH151P (IC LAB*)	6			75 marks	3
CH152P (OC LAB*)	6			75 marks	3
CH153P (PC LAB*)	6			75 marks	3
Total				**625 marks**	**25**

(*Core= compulsory papers common to all students admitted to M.ScChemistry,OU)

Semester 2

	Hrs/week	Internal assessment	Semester exam	Total	Credits
CH201T (*)	4	20 marks	80 marks	100 marks	4
CH202T (*)	4	20 marks	80 marks	100 marks	4
CH203T (*)	4	20 marks	80 marks	100 marks	4
CH204T (*)	4	20 marks	80 marks	100 marks	4
CH251P (IC LAB*)	6			75 marks	3
CH252P (OC LAB*)	6			75 marks	3
CH253P (PC LAB*)	6			75 marks	3
Total				**625 marks**	**25**

(*= compulsory papers common to all students admitted to M.ScChemistry,OU)

Semester-I and Semester-II syllabus is common for all specializations i.e., Inorganic-Analytical, Organic, Physical, Chemistry(Pharmacoinformatics) and Physical- Organic.and Pharmaceutical chemistry

M.Sc.CHEMISTRY(INORGANIC CHEMISTRY)

Syllabus for III and IV Semesters

(For the batch admitted during the academic year 2011-2012 under the CBCS pattern)

[Under Restructured CBCS Scheme]

(Approved in the P.G. BOS meeting held on 15-9-2012)

Semester - III

	Instruction	Internal assessment	Semester exam*	Total	Credits
Hrs/week	**marks**	**marks**	**marks**		
CH(IC) 301T	4	20	80	100	4
CH(IC) 302T	4	20	80	100	4
CH(IC) 303T	4	20	80	100	4
CH(IC) 304T	4	20	80	100	4
SEMINAR	2	--	--	25	1
CH(IC) 351P	9	--	100	100	4
CH(IC) 352P	9	--	100	100	4
Total				**625**	**25**

*Theory: 3 hours; Practical's: 6 hours

Semester - IV

	Instruction	Internal assessment	Semester exam*	Total	Credits
Hrs/week	**marks**	**marks**	**marks**		
CH(IC) 401T	4	20	80	100	4
CH(IC) 402T	4	20	80	100	4
CH(IC) 403T	4	20	80	100	4
CH(IC)404T (CB)	4	20	80	100	4
SEMINAR	2	--	--	25	1
CH(IC) 451P	9	--	100	100	4
CH(IC) 452P	9	--	100	100	4
Total				**625**	**25**

(**Choice based paper (CB) =** Paper offered by the same Department or other Department in the Science faculty)

*Theory: 3 hours; Practical's: 6 hours

Grand total (all 4 semesters), 2500 marks and 100 credits

M.Sc. CHEMISTRY(ORGANIC CHEMISTRY)
Syllabus for III and IV Semesters
(For the batch admitted during the academic year 2011-2012 under the CBCS pattern)

[Under Restructured CBCS Scheme]

(Approved in the P.G. BOS meeting held on 15-9-2012)

Semester - III

	Instruction	Internal assessment	Semester exam*	Total
Credits				
Hrs/week	**marks**	**marksmarks**		
CH(OC) 301T	4	20	80	100	4
CH(OC) 302T	4	20	80	100	4
CH(OC) 303T	4	20	80	100	4
CH(OC) 304T	4	20	80	100	4
SEMINAR	2	--	--	25	1
CH(OC) 351P	9	--	100	100	4
CH(OC) 352P	9	--	100	100	4
Total				**625**	**25**

*Theory: 3 hours; Practical's: 6 hours

Semester - IV

	Instruction	Internal assessment	Semester exam*	Total
Credits				
Hrs/week	**marks**	**marksmarks**		
CH(OC) 401T	4	20	80	100	4
CH(OC) 402T	4	20	80	100	4
CH(OC) 403T	4	20	80	100	4
CH(OC)404T (CB)	4	20	80	100	4
SEMINAR	2	--	--	25	1
CH(OC) 451P	9	--	100	100	4
CH(OC) 452P	9	--	100	100	4
Total				**625**	**25**

(**Choice based paper (CB) =** Paper offered by the same Department or other Department in the Science faculty)

*Theory: 3 hours; Practical's: 6 hours

Grand total (all 4 semesters) 2500 marks and 100 credits

M.Sc.CHEMISTRY(PHYSICAL CHEMISTRY)
Syllabus for III and IV Semesters
(for the batch admitted during the academic year 2011-2012 under the CBCS pattern)
[Under Restructured CBCS Scheme]
(Approved in the P.G. BOS meeting held on 15-9-2012)

Semester - III

Hrs/week	Internal assessment	Semester exam	Total	Credits
CH (P) 301T	4	20 marks	80 marks	100 marks 4
CH (P) 302T	4	20 marks	80 marks	100 marks 4
CH (P) 303T	4	20 marks	80 marks	100 marks 4
CH (P) 304T	4	20 marks	80 marks	100 marks 4
Seminar	2			25 marks 1
CH (P) 351P	9	_	100 marks	100 marks 4
CH (P) 352P	9	_	100 marks	100 marks 4
Total				**625 marks 25**

Semester - IV

	Hrs/week	Internal assessment	Semester exam	Total	Credits
CH (P) 401T	4	20 marks	80 marks	100 marks	4
CH (P) 402T	4	20 marks	80 marks	100 marks	4
CH (P) 403T	4	20 marks	80 marks	100 marks	4
CH (P) 404T (CB)	4	20 marks	80 marks	100 marks	4
Seminar	2			25 marks	1
CH (P) 451P	9	_	100 marks	100 marks	4
CH (P) 452P	9	_	100 marks	100 marks	4
Total				**625 marks**	**25**

(**Choice based paper (CB)** = Paper offered by the same Department or other Department in the Science faculty)

Grand total marks and credits (all 4 semesters) 2500 marks - 100 credits

M.Sc.CHEMISTRY(PHYSICAL ORGANIC)

Syllabus for III and IV Semesters

(For the batch admitted during the academic year 2011-2012 under the CBCS pattern)

[Under Restructured CBCS Scheme]

(Approved in the P.G. BOS meeting held on 15-9-201)

Semester - III

	Instruction	Internal assessment	Semester exam	Total	Credits
Hrs/week	**marks**	**marks**	**marks**		
CH(PO) 301T	4	20	80	100	4
CH(PO) 302T	4	20	80	100	4
CH(PO) 303T	4	20	80	100	4
CH(PO) 304T	4	20	80	100	4
SEMINAR	2			25	1
CH(PO) 351P	9	_	100	100	4
CH(PO) 352P	9	_	100	100	4
Total				**625**	**25**

*Theory: 3 hours ; Practical's: 6 hours

Semester - IV

	Instruction	Internal assessment	Semester exam	Total	Credits
Hrs/week	**marks**	**marks**	**marks**		
CH(PO) 401T	4	20	80	100	4
CH(PO) 402T	4	20	80	100	4
CH(PO) 403T	4	20	80	100	4
CH(PO) 404T (CB)	4	20	80	100	4
SEMINAR	2			25	1
CH(PO) 451P	9	_	100	100	4
CH(PO) 452P	9	_	100	100	4
Total				**625**	**25**

(**Choice based paper (CB) =** Paper offered by the same Department or other Department in the Science faculty)

*Theory: 3 hours; Practical's: 6 hours

Grand total (all 4 semesters) 2500 marks and 100 credits

M.Sc. CHEMISTRY(PARMACO INFORMATICS)

Syllabus for III and IV Semesters

(For the batch admitted during the academic year 2011-2012 under the CBCS pattern)

[Under Restructured CBCS Scheme]

(Approved in the P.G. BOS meeting held on 15-9-2012)

Semester - III

	Instruction	Internal assessment	Semester exam*	Total	Credits
Hrs/week	**marks**	**marks**	**marks**		
CH(CPI) 301T	4	20	80	100	4
CH(CPI) 302T	4	20	80	100	4
CH(CPI) 303T	4	20	80	100	4
CH(CPI) 304T	4	20	80	100	4
SEMINAR	2	--	--	25	1
CH(CPI) 351P	9	--	100	100	4
CH(CPI) 352P	9	--	100	100	4
Total				**625**	**25**

*Theory: 3 hours; Practical's: 6 hours

Semester - IV

	Instruction	Internal assessment	Semester exam*	Total	Credits
Hrs/week	**marks**	**marks**	**marks**		
CH(CPI) 401T	4	20	80	100	4
CH(CPI) 402T	4	20	80	100	4
CH(CPI) 403T	4	20	80	100	4
CH(CPI)404T (CB)	4	20	80	100	4
SEMINAR	2	--	--	25	1
CH(CPI) 451P	9	--	100	100	4
PROJECT	9	--	100	100	4
Total				**625**	**25**

(**Choice based paper (CB) =** Paper offered by the same Department or other Department in the Science faculty)

*Theory: 3 hours; Practical's: 6 hours

Grand total (all 4 semesters) 2500 marks and 100 credits

M.Sc. CHEMISTRY(ANALYTICAL CHEMISTRY)

Syllabus for III and IV Semesters

(For the batch admitted during the academic year 2011-2012 under the CBCS pattern)

[Under Restructured CBCS Scheme]

(Approved in the P.G. BOS meeting held on 15-9-2012)

Semester - III

	Instruction	Internal assessment	Semester exam*	Total
Credits				
Hrs/week	**marks**	**marksmarks**		
CH(AC) 301T	4	20	80	100	4
CH(AC) 302T	4	20	80	100	4
CH(AC) 303T	4	20	80	100	4
CH(AC) 304T	4	20	80	100	4
SEMINAR	2	--	--	25	1
CH(AC) 351P	9	--	100	100	4
CH(AC) 352P	9	--	100	100	4
Total				**625**	**25**

*Theory: 3 hours; Practical's: 6 hours

Semester - IV

	Instruction	Internal assessment	Semester exam*	Total
Credits				
Hrs/week	**marks**	**marksmarks**		
CH(AC) 401T	4	20	80	100	4
CH(AC) 402T	4	20	80	100	4
CH(AC) 403T	4	20	80	100	4
CH(AC)404T (CB)	4	20	80	100	4
SEMINAR	2	--	--	25	1
CH(AC) 451P	9	--	100	100	4
CH(AC) 452P	9	--	100	100	4
Total				**625**	**25**

(**Choice based paper (CB) =** Paper offered by the same Department or other Department in the Science faculty)

*Theory: 3 hours; Practical's: 6 hours

Grand total (all 4 semesters), 2500 marks and 100 credits

DEPARTMENT OF CHEMISTRY ,OSMANIA UNIVERSTY
M.Sc.Chemistry I &II Semester (CBCS) Syllabus
(effective from academic year 2011-2012 for Campus and Constituent colleges excluding Affiliated and District PG Centers)
[UNDER RESTRUCTURED CBCS Scheme]
(Approved in the P.G. BOS meeting held on 08-9-2011 and 15-9-2012)

Semester I

	Hrs/week	Internal assessment	Semester exam	Total	Credits
CH101T	4	20 marks	80 marks	100 marks	4
CH102T	4	20 marks	80 marks	100 marks	4
CH103T	4	20 marks	80 marks	100 marks	4
CH104T	4	20 marks	80 marks	100 marks	4
CH151P (IC LAB)	6			75 marks	3
CH152P (OC LAB)	6			75 marks	3
CH153P (PC LAB)	6			75 marks	3
Total				**625 marks**	**25**

Semester II

	Hrs/week	Internal assessment	Semester exam	Total	Credits
CH201T	4	20 marks	80 marks	100 marks	4
CH202T	4	20 marks	80 marks	100 marks	4
CH203T	4	20 marks	80 marks	100 marks	4
CH204T	4	20 marks	80 marks	100 marks	4
CH251P (IC LAB)	6			75 marks	3
CH252P (OC LAB)	6			75 marks	3
CH253P (PC LAB)	6			75 marks	3
Total				**625 marks**	**25**

Semester-I and Semester-II syllabus is common for all specializations i.e., Inorganic, Analytical, Organic, Physical, Pharmacoinformatics and Physical-Organic.and Pharmaceutical chemistry

M.Sc. CHEMISTRY (CBCS) SYLLABUS

(Effective from the academic year 2011-2012 for Campus and Constituent colleges excluding affiliated and district PG Centers)

SEMESTER –I

Paper-I: CH 101T (INORGANIC CHEMISTRY)

IC 01: Symmetry of molecules
IC 02: Bonding in Metal Complexes - I
IC 03: Coordination equilibria
IC 04: Ligational aspects of diatomic molecules

IC-01: Symmetry of Molecules:

Concept of Symmetry in Chemistry – Symmetry Operations – Symmetry Elements : Rotational Axis of Symmetry and Types of Rotational Axes, Plane of Symmetry and types of Planes, Improper Rotational Axis of Symmetry , Inversion Center and Identity Element – More about Symmetry Elements – Molecular Point Groups: Definition and Notation of Point Groups, Classification Molecules in to C_1, C_s , C_i , C_n ,C_{nv} , C_{nh} , $C_{\infty v}$, D_n , D_{nh} , D_{nd} ,$D_{\infty h}$, S_n (n=even), T ,T_h , T_d , O , O_h , I, I_h , K_h Groups. Descent in Symmetry with Substitution – Exercises in Molecular Point Groups – Symmetry and Dipole moment – Symmetry criteria for Optical activity..

IC – 02: Bonding in metal complexes – I:

Crystal Field Theory: Salient features of CFT. d-orbital splitting patterns in regular Octahedral, tetragonally distorted octahedral, Jahn-Tellar theorem-, tetrahedral, square planar, trigonal planar, and linear geometries. Factors influencing the magnitude of crystal field splitting in octahedral complexes – nature of metal ions, nature of ligands, geometry. Concept of weak field and strong fields. - Calculation of crystal field stabilization energies (CFSE's) in six and four coordinate complexes.

Types of magnetic behaviour – magnetic susceptibility – calculation of magnetic moment from magnetic susceptibility spin only formula ,- Quenching of orbital angular momentum – Determination of magnetic moment from Guoy's method . Applications of magnetic moment data for the determination of oxidation states, bond type and stereochemistry.

IC-03: Coordination Equilibria:

Solvation of metal ions- Binary complexes: Formation of binary Metal Complexes and their stability – types of Stability Constants – relation between them- trends in Step-wise Stability Constants (Factors causing decrease and increase in Step-wise Stability) – Factors influencing the stability constants : (i) Ligand effects: Basicity , Substituent , Steric

,Chelate(size and number of chelate rings) , Macrocyclic and Cryptate effects- (ii) Metal ion effects: Ionic potential ,Effective Nuclear charge and Atomic Number (Irving-William's Order, geometry of Metal ion and Ligand) – Chelate effect and its Thermodynamic origin – Jahn-Tellar effect on Stability constants of Metal complexes – Pearson's Theory of Hard and Soft Acids and Bases (HSAB) , Applications of HSAB, Electronegetivity Vs Hardness and Softness. Symbiosis – Methods used for the determination of Stability constants (Basic Principles only): pH metric, Spectrophotometric and Polarographic methods.
Ternary Metal Complexes – definition – Formation of ternary metal complexes – Step-wise and simultaneous equilibria with simple examples.

IC – 04: Ligational Aspects of Diatomic molecules:

Metal Carbonyls:- Carbon monoxide as a ligand – Molecular orbitals of CO - Donor and Acceptor molecular orbitals of CO; Bonding modes of CO- Terminal and Bridging; Evidence for multiple bonding from Bond lengths and Stretching frequencies;
18 Valence electron rule and its application.
Metal Nitrosyls: - NO as a ligand – Molecular orbitals of NO – Donor and Acceptor components; Bonding modes of NO – Terminal (Linear, Bent) and Bridging;
Structural aspects of $[IrCl(PPh_3)_2(CO)(NO)]^+$ and $[RuCl(PPh_3)_2(NO)_2]^+$.
Stereo chemical control of valence in $[Co(diars)_2(NO)]^{2+}$ and $[Co(diars)_2(NO)(SCN)]^+$.
Metal Dinitrogen complexes: - N_2 as aligand – Molecular orbitals of N_2; Bonding modes – Terminal and Bridging; Stretching frequencies; Structures of Ru (II) and Mo (0) dinitrogen complexes; Chemical fixation of dinitrogen.

Suggested References:

1. Symmetry and Group theory in Chemistry, Mark Ladd, Marwood Publishers, London (2000).
2. Molecular Symmetry and Group Theory, Robert L.Carter, John Wiley & Son (1998).
3. Symmetry and Spectroscopy of Molecules. K.Veera Reddy, New Age International (P) Limited (1999).
4. Advanced Inorganic Chemistry. F.A.Cotton, G.Wilkinson, C.A.Murillo and M.Bochmann, 6 th Edition, Wiley Interscience, N.Y (1999
5. Inorganic Chemistry, J.E.Huheey , K.A.Keiter and R.L.Keiter 4 th Edition Harper Cottens College Publications (1993).
6. Homogeneous Catalysis by Metal complexes Vol I, M M Taqui Khan and A E Martell, Academic Press NY (1974).
7. Inorganic Chemistry, Keith F.Purcell and John C.Kotz, Holt-Saunders International Editions, London (1977).

Paper-II: CH 102 T(ORGANIC CHEMISTRY)

OC-01: Stereochemistry
OC-02: Reaction mechanism-I
OC-03: Carbohydrates and Proteins
OC-04: Heterocyclic compounds

OC-01: Stereochemistry

Molecular representations: Wedge, Fischer, Newman and Saw-horse formulae, their description and interconversions.

Molecular Symmetry & Chirality: Symmetry operations and symmetry elements (Cn & Sn). Criteria for Chirality. Desymmetrization.

Axial, planar and helical chirality: Configurational nomenclature:Axially chiral allenes,spiranes,alkylidene cycloalkanes, chiral biaryls, atropisomerism.Planar chiral ansa compounds and trans- cyclooctene.Helically chiral compounds

Relative and absolute configuration: Determination of absolute configuration by chemical correlation methods.

Racemisation, racemates and resolution techniques: Resolutions by direct crystallization, diastereoisomer salt formation chiral chromatography and asymmetric transformation.

Determination of configuration in E,Z-isomers: Spectral and Chemical methods of configuration determination of E,Z isomers. Determination of configuration in aldoximes and ketoximes.

OC-02: Reaction mechanism-I

Electrophilic addition to carbon carbon double bond: Stereoselective addition to carbon carbon double bond ; *anti* addition- Bromination and epoxidation followed by ring opening. *Syn* addition of OsO_4 and $KMnO_4$.

Elimination reactions Elimination reactions E2, E1, E1CB mechanisms. Orientation and stereoselectivity in E2 eliminations. Pyrolytic *syn* elimination and α-elimination, elimination Vs substitution.

Determination of reaction mechanism: Determination of reaction mechanism: Energy profiles of addition and elimination reactions, transition states, product isolation and structure of intermediates, use of isotopes, chemical trapping, crossover experiments. Use of IR and NMR in the investigation of reaction mechanism.

OC-03: Carbohydrates and Proteins

Carbohydrates: Determination of the relative and absolute configuration in D (+) glucose and D (-) fructose.Proof for the chair conformation of D (+) glucose. Occurence, importance and synthesis of monosaccharides containing functional groups such as amino, halo and sulphur. Structure elucidation and synthesis of sucrose.Conformational structures of D(+)ribose, 2-deoxyD-ribose, sucrose, lactose maltose and cellobiose. Structural features of starch, cellulose and chitin.

Proteins: Acid and enzymatic hydrolysis of proteins.Determination of the amino acid sequence in polypeptides by end group analysis.Chemical synthesis of di and tripeptides. Merrifield's solid phase synthesis.

OC-4: Heterocyclic compounds

Importance of heterocyclic compounds as drugs. Nomenclature of heterocyclic systems based on ring size,number and nature of hetero atoms.Synthesis and reactivity of indole, benzofuran, benzothiophene, quinoline, isoquinoline, coumarin, chromone, carbazole and acridine.

References:

1. Stereochemistry of carbon compounds by Ernest L.Eliel and Samuel H. Wilen
2. Stereochemistry of organic compounds- Principles and Applications by D. Nasipuri
3. Heterocyclic Chemistry, T.L. Gilchrist, Longman UK Ltd, London (1985).
4. Benzofurans A. Mustafa, Wiley-Interscience, New York (1974).
5. Heterocyclic Chemistry, 3rd Edn J.A.Joule, K.Mills and G..F.Smith, Stanley Thornes Ltd,UK, (1998)
6. The Chemistry of Indole, R.J. Sunderberg, Academic Press, New York (1970).
7. An introduction to the chemistry of heterocyclic compounds, 2nd Edn.R.M.Acheson, Interscience Publishers, New York, 1967.
8. Advanced Organic Chemistry by Jerry March
9. Mechanism and Structure in Organic Chemistry S. Mukerjee
10. Guide Book to mechanism in Organic Chemistry, 6th Edition, Peter Sykes.
11. Organic Chemistry by Graham Solomous and Craig Fryhle.
12. Organic Chemistry by RT Morrison and RN Boyd.
13. Organic Chemistry, Vol. 2 by I.L. Finar.
14. Organic Chemistry: Structure and Reactivity by Seyhan Ege.

Paper-III: CH 103 T(PHYSICAL CHEMISTRY)

PC-01: Thermodynamics-I
PC-02: Electrochemistry-I
PC-03: Quantum Chemistry-I
PC-04: Chemical Kinetics-I

PC-01: Thermodynamics-I

Brief review of concepts of I and II laws of thermodynamics. Concept of entropy. Entropy as a state function. Calculation of entropy changes in various processes. Entropy changes in an ideal gas. Entropy changes on mixing of ideal gases. Entropy as a function of V and T.

Entropy as a function of P and T. Entropy change in isolated systems- Clausius inequality. Entropy change as criterion for spontaneity and equilibrium.
Third law of thermodynamics. Evaluation of absolute entropies from heat capacity data for solids, liquids and gases. Standard entropies and entropy changes of chemical reactions. Helmholtz and Gibbs free energies (A and G). A and G as a criteria for equilibrium and spontaneity. Physical significance of A and G. Driving force for chemical reactions- relative signs of ΔH and ΔS.
Thermodynamic relations. Gibbs equations. Maxwell relations. Temperature dependence of G. Gibbs- Helmholtz equation. Pressure dependence of G.
Chemical potential: Gibbs equations for non-equilibrium systems. Material equilibrium. Phase equilibium. Clapeyron equation and Clausius-Clapeyron equation .
Conditions for equilibrium in a closed system. Chemical potential of ideal gases. Ideal-gas reaction equlibrium-derivation of equilibrium constant. Temperature dependence of equilibrium constant-the van't Hoff equation.

PC-02: Electrochemistry- I

Electrochemical Cells : Derivation of Nernst equation – problems. Chemical and concentration cells (with and without transference). Liquid junction potential – derivation of the expression for LJP – its determination and elimination**.** Applications of EMF measurements : Solubility product, potentiometric titrations, determination of transport numbers, equilibrium constant measurements.
Decomposition potential and its significance. Electrode polarization – its causes and elimination. Concentration overpotential.
Concept of activity and activity coefficients in electrolytic solutions. The mean ionic activity coefficient. Debye-Huckel theory of electrolytic solutions. Debye-Huckel limiting law (derivation not required). Calculation of mean ionic activity coefficient. Limitations of Debye-Huckel theory. Extended Debye-Huckel law.
Theory of electrolytic conductance. Derivation of Debye-Huckel-Onsager equation – its validity and limitations.
Concept of ion association – Bjerrum theory of ion association (elementary treatment) - ion association constant – Debye-Huckel-Bjerrum equation.

PC-03: Quantum Chemistry- I

Black body radiation-Planck's concept of quantization-Planck's equation, average energy of an oscillator (derivation not required). Wave particle duality and uncertain principle- significance of these for microscopic entities. Emergence of quantum mechanics. Wave mechanics and Schroedinger wave equation.
Operator**s**-operator algebra. Commutation of operators, linear operators.Complex functions. Hermitian operators. Operators ∇ and ∇^2 . Eigenfunctions and eigenvalues. Degeneracy.

Linear combination of eigenfunctions of an operator. Well behaved functions. Normalized and orthogonal functions.

Postulates of quantum mechanics. Physical interpretation of wave function. Observables and operators. Measurability of operators. Average values of observables. The time dependent Schrodinger equation. Separation of variables and the time-independent Schrodinger equation..

Theorems of quantum mechanics. Real nature of the eigen values of a Hermitian operator-significance. Orthogonal nature of the eigen values of a Hermitian operator-significance of orthogonality. Expansion of a function in terms of eigenvalues. Eigen functions of commuting operators-significance. Simultaneous measurement of properties and the uncertainty principle.

PC-04:Chemical Kinetics- I

Theories of reaction rates : Collision theory, steric factor. Tranition state theory. Reaction coordinate, activated complex and the transition state. Thermodynamic formulation of transition state theory. Activtion parameters and their significance. The Eyring equation. Unimolecular reactions and Lindamann's theory.

Complex reactions- Opposing reactions, parallel reactions and consecutive reactions(all first order type). Chain reactions-general characteristics, steady state treatment. Example- H_2-Br_2 reaction. Derivation of rate law.

Effect of structure on reactivity- Linear free energy relationships. Hammett and Taft equations-substituent(σ and σ^*) and reaction constant (ρ and ρ^*)with examples. Deviations from Hammett correlations. reasons- Change of mechanism, resonance interaction. Taft four parameter equation. Correlations for nucleophillic reactions. The Swain – Scott equation and the Edward equation.

The reactivity-selectivity principle and the isoselectivty rule. The intrinsic barrier and Hammond's postulate.

References:

1. Atkin's Physical Chemistry, Peter Atkins and Julio de Paula, Oxford University press
2. Physical Chemistry, Ira N. Levine, McGraw Hill
3. Physical Chemistry-A Molecular approach, D.A. McQuarrie and J.D. Simon, Viva Books Pvt. Ltd
4. Molecular Thermodynamics, D.A. McQuarrie and J.D. Simon, University Science Books
5. Quantum Chemistry, Ira N. Levine, Prentice Hall
6. Introduction to Quantum Chemistry, A.K. Chandra, Tata McGraw Hill
7. Chemical Kinetics, K.J. Laidler, McGraw Hill
8. Kinetics and Mechanism of Chemical Transformations, J. Rajaraman and J. Kuriacose, McMillan
9. Introduction to Electrochemistry, S. Glasstone
10. Modern Electrochemistry, J. O. M. Bockris & A. K. N. Reddy, Plenum

11. Principles of physical chemistry, Samuel H. Maron and Carl F. Prutton, Oxford& IBH
12. The Physical Basis of Organic Chemistry by Howard Maskill, Oxford University Press (New York)
13. Chemical Kinetics and Reaction Mechanisms, J. H. Espenson, McGraw Hill
14. Physical Organic Chemistry, N. S. Isaacs, ELBS

Paper-IV: CH 104 T (ANALYTICAL TECHNIQUES and SPECTROSCOPY- I)

ASP 01: Techniques of Chromatography
ASP 02: NMR spectroscopy-I (^{1}H NMR)
ASP 03: Rotational and Vibrational spectroscopy
ASP 04: Electronic spectroscopy

ASP-01: Techniques of Chromatography

i. Introduction, Classification of chromatographic techniques, differential migration rates, partition ratio, retention time, relation between partition ratio and retention time, capacity factor, selectivity factor. Efficiency of separation- resolution, diffusion, plate theory and rate theory.

ii. **GC:** Principle, instrumentation, detectors- TCD, FID, ECD. Derivatisation techniques, PTGC.

iii. **HPLC:** Principle, instrumentation, detectors- UV detectors, Photodiode array detector, fluorescence detector.

iv. Applications: Methods of quantitation for GC and HPLC: GC analysis of hydrocarbons in a mixture, GC assay of methyl testosterone in tablets, atropine in eye drops. HPLC assy of paracetamol and asprin in tablets.

ASP 02: NMR spectroscopy-I (^{1}H NMR)

^{1}H NMR spectroscopy: Magnetic properties of nuclei, Principles of NMR. Instrumentation, CW and pulsed FT instrumentation, equivalent and non equivalent protons, enantiotopic and diastereotopic protons, Chemical shifts, factors affecting the chemical shifts, electronegativity and anisotropy, shielding and deshielding effects,Signal integration, Spin-spin coupling: vicinal,germinal and long range, Coupling constants and factors affecting coupling constants. Applications of ^{1}H NMR spectroscopy: Reaction mechanisms (cyclic bromonium ion,electrophilic and nucleophilic substitutions, carbocations and carbanions),E,Z isomers,conformation of cyclohexane and decalins, keto-enol tautomerism, hydrogen bonding, proton exchange processes (alcohols, amines and carboxylic acids), C-N rotation. Magnetic resonance imaging(MRI). ^{1}H NMR of organic molecules and metal complexes:

ethyl acetate, 2- butanone, mesitylene, paracetamol, asprin, ethylbenzoate, benzyl acetate, 2-chloro propionic acid, $[HNi(OPEt_3)_4]^+$, $[HRh(CN)_5]$ Rh I=1/2, $[Pt(acac)_2]$.

ASP 03 :Rotational and Vibrational spectroscopy

a). Microwave Spectroscopy: Classification of molecules based on moment of inertia. Diatomic molecule as rigid rotator and its rotational energy levels. Selection rules (derivation not required). Calculation of bondlengths from rotational spectra of diatomic molecules. Isotope effect on rotational spectra. Calculation of atomic mass from rotational spectra. Brief description of microwave spectrometer.

b). Vibrational Spectroscopy. Vibrational energy levels of diatomic molecules, selection rules (derivation not required). Calculation force constant from vibrational frequency. Anharmonic nature of vibrations. Fundamental bands, overtones and hot bands, Fermi Resonance. Vibration-rotation spectra diatomic molecules. Vibrations of poly atomic molecules. Normal modes of vibration, concept of group frequencies. Characteristics of vibrational frequencies of functional groups; Stereochemical effects on the absorption pattern in carbonyl group, cis-trans isomerism and hydrogen bonding. Isotopic effect on group frequency. IR spectra of metal coordinated NO_3^-, SO_4^{2-} and CO_3^{2-} ions.

Raman Spectroscopy- Quantum theory of Raman effect, Rotational raman and Vibrational Raman spectra, Stokes and anti- Stokes lines. Complementary nature of IR and Raman spectra.

ASP 04:Electronic spectroscopy

Electronic spectroscopy: Electronic spectra: Elementary energy levels of molecules-selection rules for electronic spectra; types of electronic transitions in molecules. Chromophores: Congugated dienes, trienes and polyenes, unsaturated carbonyl compounds, benzene and its derivatives, Woodward-Fieser rules. Polynuclear aromatic hydrocarbons and diketones. Solvent and structural influences on absorption maxima, stereochemical factors. Cis-trans isomers, and cross conjugation. Beer's law application to mixture analysis and dissociation constant of a weak acid.

References:

1. Fundamentals of Molecular Spectroscopy, Banwell and McCash.
2. Introduction to Molecular Spectroscopy, G.M. Barrow.
3. Absorption Spectroscopy of Organic Compounds, J.R. Dyer.
4. Biochemistry: Hames and Hooper.
5. Introduction to Spectroscopy, Pavia Lampman Kriz.
6. Pharmaceutical analysis, Watson
7. NMR in Chemistry- A multinuclear introduction, William Kemp.
8. Organic Spectroscopy, William Kemp.

9. Spectroscopy of organic compounds, P.S. Kalsi.
10. Structural methods n Inorganic chemistry, E.A.V Ebsworth.

Paper CH 151P: Inorganic Chemistry Practicals: 6 hrs/week

I. Calibrations:
(i) Calibration of weights.
(ii) Calibration of pipettes.
(iii) Calibration of standard flasks.
(iv) Calibration of burette.
II. EDTA back-titrations:
(i) Estimation of Ni^{2+}.
(ii) Estimation of Al^{3+}.
III. EDTA substitution titrations:
Estimation of Ca^{2+}.
IV. Preparation of complexes:
(i). Hexaammine nickel (II) chloride.
(ii). Tris (acetylacetanato) manganese.
(iii). Tris (ethylenediamine) nickel (II) thiosulphate.
(iv). Mercury tetrathiocyanato cobaltate (II).
V. Preparation of complexes and calculation of % purity:
(i). Tetrammine copper (II) sulphate and estimation of NH_3 and calculation of % purity.
(ii). Pentaammine (chloro) cobalt (III) chloride and estimation of Cl^- and calculation of % purity.
(iii). Sodium trioxalato ferrate (III) and estimation of $C_2O_4^{2-}$ and Fe^{2+} and calculation of % purity.

Paper CH 152P Organic Chemistry Lab course : 6 hrs / week

Synthesis of the following compounds: p-Bromoacetanilide (using Ceric ammonium nitrate and KBr), p- Bromoaniline, 2,4,6- tribromoaniline, 1,3,5-tribromobenzene, tetrahydrocarbazole, 7-hydroxy-4-methylcoumarin, m-dinitrobenzene, m-nitroaniline, hippuricacid, azlactone, anthracene-maleicanhydride adduct, phthalimide, 2,4-dihydroxyacetophenone and dihydropyrimidinone (using Ethylacetoacetate , Benzaldehyde and Urea).

References.

1. Text book of practical organic chemistry, Vogel
2. Text book of practical organic chemistry, Mann and Saunders.

Paper 153P Physical Chemistry Lab course : 6 hrs / week

Physical properties: Determination of density, surface tension and viscosity of liquids

Distribution:

- Distribution of acetic acid between n-butanol and water
- Distribution of iodine between CCl_4 and water

Chemical kinetics:

- Acid-catalyzed hydrolysis of methyl acetate
- Peroxydisulphate- I^- reaction (overall order)
- Oxidation of iodide ion by hydrogen peroxide- iodine clock reaction

Conductometry:

- Titration of strong acid vs strong base
- Titration of weak acid vs strong base
- Determination of cell constant
- Determination of dissociation constant of a weak acid

Potentiometry:

- Titration of strong acid vs strong base
- Titration of weak acid vs strong base
- Determination of dissociation constant of a weak acid
- Determination of single electrode potential

Polarimetry:

- Determination of specific rotation of sucrose
- Acid-catalyzed hydrolysis of sucrose (inversion of sucrose)

Adsorption and others:

- Adsorption of acetic acid on animal charcoal or silica gel
- Determination of critical solution temperature of phenol-water system
- Effect of added electrolyte on the CST of phenol-water system

SEMESTER –II

Paper-I: CH 201T (INORGANIC CHEMISTRY)

IC 05: Reaction mechanisms of transition metalcomplexes
IC 06: Bonding in metal complexes-II
IC 07: Metal clusters
IC 08: Biocoordination chemistry

IC-05: Reaction mechanisms of transition metal complexes:

Ligand substitution reactions:
Energy profile of a reaction – Transition state or Activated Complex. Types of substitution reactions (SE,SN,SN^1,SN^2).
Ligand substitution reactions in octahedral complexes:
Aquation or Acid hydrolysis reactions, Factors effecting Acid Hydrolysis , Base Hydrolysis, Conjugate Base Mechanism, Evidences in favour of SN^1CB Mechanism.
Annation reactions.
Substitution reactions with out Breaking Metal-Ligand bond.
Ligand Substitution reactions in Square-Planar complexes: Mechanism of Substitution in Square-Planar complexes- Trans-effect, Grienberg's Polarization theory and π - bonding theory – Applications of Trans-effect in synthesis of Pt (II) complexes.
Electron Transfer Reactions (or Oxidation-Reduction Reactions) in Coordination compounds:
Mechanism of One-electron Transfer Reactions: Atom (or group) Transfer or Inner Sphere Mechanism, Direct electron Transfer or Outer Sphere Mechanism. Marcus –Hush theory.

IC-06: Bonding in Metal Complexes – II:

Free ion terms and Energy levels: Configurations,Terms,States and Microstates – Formula for the calculation of Microstates p^n and d^n configurations – L-S (Russel-Saunders) coupling scheme – j-j coupling scheme – Determination of terms for various p^n and d^n configurations of metal ins. Hole formalism – Energy ordering of terms (Hund's rules) Inter – electron repulsion Parameters (Racah parameters) – Spin-Orbital coupling parameters. Effect of weak cubic crystal fields on S,P,D and F terms- Orgel Diagrams.Jahn –Tellor theorem and its effects on terms.

IC-07: Metal Clusters:

Carbonyl clusters: Factors favouring Metal-Metal bonding – Classification of Clusters – Low Nuclearity Clusters : M_3 and M_4 clusters , structural patterns in $M_3(CO)_{12}$ (M=Fe,Ru,Os) and $M_4(CO)_{12}$ (M=Co,Rh,Ir) Clusters-. Metal carbonyl scrambling – High Nuclearity clusters M_5,M_6,M_7,M_8 and M_{10} Clusters-, Polyhedral skeletal electron pair theory and Total Electron Count theory – Wades rules – Capping rule – Structural patterns in $[Os_6(CO)_{18}]^{2-}$, $[Rh_6(CO)_{16}]$, $[Os_7(CO)_{21}]$, $[Rh_7(CO)_{16}]^{3-}$, $[Os_8(CO)_{22}]^{2-}$, $[Os_{10}C(CO)_{24}]^{2-}$ and $[Ni_5(CO)_{12}]^{2-}$.
Metal Halide clusters: Major structural types in Dinuclear Metal-Metal systems – Edge sharing Bioctahedra,Face sharing Bioctahedra,Tetragonal prismatic and Trigonal antiprismatic structures -. Structure and bonding in $[Re_2Cl_8]^{2-}$ and Octahedral halides of $[Mo_6(Cl)_8]^{4+}$ and $[Nb_6(Cl)_{12}]^{2+}$. Trinuclear halides of Re(III).Hoffman's Isolobal analogy and its Structural implications.

IC-08: Bio Coordination Chemistry:

Metal ions in Biological systems: Brief survey of metal ions in biological systems. Effect of metal ion concentration and its physiological effects. Basic principles in the biological selection of elements.

Oxygen transport and storage: Hemoglobin and Myoglobin: Geometric, electronic and magnetic aspects of Dioxygen binding, Oxygen adsorption isotherms and cooperativity in Hemoglobin and its physiological significance. Role of globin chain. Hemerythrin and Hemocyanin: Structure of deoxy forms, oxygen binding, Geometric, electronic and magnetic aspects. Comparison of Hemerythrin and Hemocyanin with hemoglobin.

Photosynthesis: Structural aspects of Chlorophyll. Photo system I and Photo system II.

Vitamin B_6 model systems: Forms of vitamin B_6 with structures. Reaction mechanisms of (1) Transamination (2) Decarboxylation and (3) Dealdolation in presence of metal ions.

References:

1. Inorganic Reaction Mechanisms. M.L.Tobe and John Burgess, Addison Wesley Longman (1999).
2. Metal ions in Reaction Mechanisms. K.Veera Reddy. Golgotia Publications (P) Ltd
3. Mechanisms of Reactions in Transition Metal Sites. Richard A Henderson, Oxford Science Publications, London (1993).
4. Inorganic Reaction Mechanisms, F.Basolo and R.G.Pearson, New York (1967).
5. Advanced Inorganic Chemistry. F.A.Cotton, G.Wilkinson, C.A.Murillo and M.Bochmann, 6 Th Edition, Wiley Interscience, N.Y (1999
6. Inorganic Chemistry, J.E.Huheey , K.A.Keiter and R.L.Keiter 4 th Edition Harper Cottens College Publications (1993).
7. Inorganic Biochemistry Edited by G.L.Eichorn, Volume 1 Elsevier (1982).
8. The Chemistry of Metal Cluster Complexes. D.F.Shriver, H.D.Kaerz and R.D.Adams (Eds), VCH, NY (1990).
9. Inorganic Chemistry, Keith F.Purcell and John C.Kotz, Holt-Saunders International Editions, London (1977).
10. Bioinorganic Chemistry, I.Bertini, H.B.Gray, S.J.Lippard and S.J.Valentine, Viva Low-Priced Student Edition, New Delhi (1998).
11. Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, W.Kain and B.Schwederski, John Wiley and Sons, NY (1999).
12. Bioorganic Chemistry – Dugas.

Paper-II: CH 202T (ORGANIC CHEMISTRY)

OC-05: Conformational analysis (acyclic systems)
OC-06: Reaction mechanism-II
OC-07: Reactive intermediates and Molecular rearrangements.
OC-08: Natural products (Terpenoids and Alkaloids).

OC-05: Conformational analysis (acyclic systems)

Introduction to conformational isomerism and the concept of dynamic stereochemistry.Study of conformations in ethane and 1,2-disubstituted ethane derivatives like butane, dihalobutanes, halohydrin, ethylene glycol, butane-2, 3-diol amino alcohols and 1,1,2,2-tetrahalobutanes. Klyne-Prelog terminology for conformers and torsion angles Conformations of unsaturated acyclic compounds-Propylene,
1-Butene, Acetaldehyde, Propionaldehyde and Butanone. Conformational diastereoisomers and conformational enantiomers -. Factors affecting the conformational stability and conformational equilibrium – Attractive and repulsive interactions. Use of Physical and Spectral methods in conformational analysis.
Conformational affects on the stability and reactivity of acyclic diastereoisomers – steric and stereoelectronic factors-examples.Conformation and reactivity: The Winstein-Holness equation and the Curtin – Hammett principle.

OC-06: Reaction mechanism-II

Nucleophilic Aromatic substitution: Aromatic Nucleophilic substitution: $S_N1(Ar)$, S_N2 (Ar), and benzyne mechanisms; evidence for the structure of benzyne. Von Richter rearrangement. Definition and types of ambident nucleophiles.
Neighbouring group participation : Criteria for determining the participation of neighbouring group. Enhanced reaction rates, retention of configuration, isotopic labeling and cyclic intermediates. Neighbouring group participation involving Halogens, Oxygen, Sulphur, Nitrogen, Aryl, Cycloalkyl groups, σ and π- bonds. Introduction to nonclassical carbocations.
Electrophilic substitution at saturated carbon and single electron transfer reactions.
Mechanism of aliphatic electrophilic sustitution. S_E1, S_E2, and S_Ei. SET mechanism.

OC-07: Reactive intermediates and Molecular rearrangements.

Reactive Intermediates: Generation, detection, structure, stability and reactions of carbocations, carbanions, carbenes, nitrenes and free radicals.
Molecular rearrangements: Definition and classification. Molecular rearrangements involving 1) electron deficient carbon: Wagner- Meerwein, Pinacol-Pinacolone, Allylic and Wolf rearrangement. 2) electron deficient Nitrogen: Hofmann, Lossen, Curtius, Schmidt and Beckmann rearrangements 3) electron deficient Oxygen: Baeyer-Villiger oxidation. 4) Base catalysed rearrangements: Benzilic acid , Favourski , Transannular , Sommlett-Hauser and Smiles rearrangement

OC-08: Natural products-I (Terpenoids and Alkaloids)

Importance of natural products as drugs. Isolation of natural products by steam distillation, solvent extraction and chemical methods. General methods in the structure determination of terpenes. Isoprene rule. Structure determination and synthesis of α-terpeniol and camphor. Biogenesis of monoterpenes. Structure determination and synthesis of β-carotene. General methods of structure determination of alkaloids. Structure determination and synthesis of papaverine and quinine.

References :

1. Stereochemistry of Carbon compounds by Ernest L Eliel / Samuel H. Wilen
2. Stereochemistry of organic compounds – Principles and Applications by D Nasipuri
3. The third dimension in organic chemistry, by Alan Bassindale
4. Stereochemistry: Conformation and Mechanism by P S Kalsi
5. Stereochemistry by V M Potapov
6. Advanced Organic Chemistry by Jerry March
7. Mechanism and Structure in Organic Chemistry S. Mukerjee
8. Organic chemistry Vol.I and II by I.L.Finar
9. Comprehensive organic chemistry Vol.5 D.H.R.Barton and W.D..Ollis
10. Organic Chemistry, Vol. 2 by I.L. Finar.
11. Chemistry of Natural Products by Bhat, Nagasampagi and Siva Kumar.
12. Alkaloids by K.W. Bentley.
13. Steroids and Terpenoids by Bentle.

Paper-III: CH 203T (PHYSICAL CHEMISTRY)

PC-05: Thermodynamics-II
PC-06: Photochemistry-I
PC-07: Quantum Chemistry-II
PC-08: Solid state chemistry

PC-05:Thermodynamics-II

Solutions: Specifiying the Solution composition. Partial molar poperties-significance. Relation between solution volume and partial molar volume. Measurement of partial molar volumes- slope and intercept methods. The chemical potential. Variation of chemical potential with T and P. Gibbs-Duhem equation-derivation and significance

Ideal solutions. Thermodynamic properties of ideal solutions. Mixing quantities. Vapour pressure-Raoult's law. Thermodynamic properties of ideally dilute solutions. Vapour pressure- Henry's law.

Nonideal systems. Concept of fugacity, fugacity coefficeient. Determination of fugacity. Non ideal solutions. Activities and activity coefficients. Standard-state conventions for non ideal solutions. Determination of activity coefficients from vapour pressure measurements. Activity coefficients of nonvolatile solutes using Gibbs-Duhem equation.

Multicomponent phase equilibrium: Vapour pressure lowering, freezing point depression and boiling point elevation

PC-06:Photochemistry –I

Electronic transitions in molecules. The Franck Condon principle. Electronically excited molecules- singlet and triplet states. Radiative life times of excited states-theoretical treatment. Measured lifetimes. Quantum yield and its determination. Actinomety-ferrioxalate and uranyl oxalate actinometers-problems.

Derivation of fluorescence and phosphorescence quantum yields. E-type delayed fluorescence- evaluation of triplet energy splitting(ΔE_{ST}). Photophysical processes-photophysical kinetics of unimolecular reactions. Calculation of rate constants of various photophysical processes-problems, State diagrams

Photochemical primary processes. Types of photochemical reactions- electron transfer, photodissociation, addition, abstraction, oxidation and isomerization reactions with examples. Effect of light intensity on the rates of photochemical reactions. Photosensitization. Quenching-Stern Volmer equation. Experimental set up of a photochemical reaction. Introduction to fast reactions- Principle of flash photolysis.

PC-07: Quantum chemistry-II

Particle in a box- one dimensional and three dimensional. Plots of ψ and ψ^2-discussion. Degeneracy of energy levels. Comparison of classical and quantum mechanical particles. Calculations using wave functions of the particle in a box-orthoganality, measurability of energy, position and momentum, average values and probabilities. Application to the spectra of conjugated molecules.

Cartesian, Polar and spherical polar coordinates and their interrelations

Schrodinger equation for the hydrogen atom- separation into three equations. Hydrogen like wave functions. Radial and angular functions. Quantum numbers n, l and m and their importance. The radial distribution functions. Hydrogen like orbitals and their representation. Polar plots, contour plots and boundary diagrams.

Many electron systems. Approximate methods. The variation method-variation theorem and its proof. Trial variation function and variation integral. Examples of variational calculations.

Paricle in a box. Construction of trial function by the method of linear combinations. Variation parameters. Secular equations and secular determinant..

Bonding in molecules. Molecular orbital theory-basic ideas. Construction of MOs by LCAO , H_2^+ ion. The variationan integral for H_2^+ ion. Detailed calculation of Wave functions and energies for the bonding and antibonding MOs. Physical picture of bonding and antibonding wave functions. Energy diagram. The MO and VB wave functions for H_2 molecule and their comparision.

PC-08: Solid state chemistry

Magnetic properties of solids- classification of magnetic materials, Magnetic susceptibility, Langevin diamagnetism, Weiss theory of para magnetism

Electronic properties of metals, insulators and semi conductors: Electronic structure of solids, Band theory, band structure of metals, insulators and semiconductors. Electrons, holes and Excitons. The temperature dependence of conductivity of extrinsic semi conductors. Photo conductivity and photovoltaic effect-p-n junctions.

Superconductivity. Occurrence of superconductivity. Destruction of superconductivity by magnetic fields-Meisner effect. Types of superconductors. Theories of super conductivity-BCS theory.

High temperature superconductors. Structure of defect perovskites. High T_c superconductivity in cuprates. Phase diagram of Y-Ba-Cu-O system. Crystal structure of $YBa_2Cu_3O_{7-x}$. Preparation of 1-2-3 materials. Origin of high T_c superconductivity.

References:

1. Atkin's Physical Chemistry, Peter Atkins and Julio de Paula, Oxford University press
2. Physical Chemistry, Ira N. Levine, McGraw Hill
3. Physical Chemistry-A Molecular approach, D.A. McQuarrie and J.D. Simon, Viva Books Pvt Ltd
4. Molecular Thermodynamics, D.A. McQuarrie and J.D. Simon, University Science Books
5. Quantum Chemistry, Ira N. Levine, Prentice Hall
6. Introduction to Quantum Chemistry, A.K. Chandra, Tata McGraw Hill
7. Introduction to Solids, Leonid V. Azaroff, Tata McGraw Hill
8. Solid state Chemistry, D.K. Chakrabarthy, New Age International
9. Solid state Chemistry and its aplications, A.R. West, Plenum.
10. Fundamentals of Photochemistry, K.K.Rohtagi-Mukherji, Wiley-Eastern
11. Molecular Photochemistry, N.J. Turro, Benjamin
12. Photochemistry, R.P.Kundall and A. Gilbert, Thomson Nelson

13. Essentials of Molecular Photochemistry by A. Gilbert and J. Baggott, Blackwell Scientific Publications.
14. Organic Photochemistry by J.M.Coxon and B.Halton, Cambridge University press.
15. Introductory Photochemistry by A.Cox and T.J.Kemp. McGraw-Hill, London.
16. Principles of the Solid State, H. V. Keer, New Age International

Paper-IV: CH 204 T(ANALYTICAL TECHNIQUES and SPECTROSCOPY - II)

ASP-05: Electro analytical Techniques.
ASP-06: NMR- II
ASP-07: Mass Spectroscopy
ASP-08: Photoelectron & ESR spectroscopy

ASP-05: Electro Analytical Techniques

a) Types and Classification of Electro analytical Methods.

i) Potentiometry- Types of electrodes, Hydrogen gas, Calomel, Quin hydrone and glass electrodes. Determination of pH. Potentiometric titrations.

ii) Conductometry – Definition of terms – conductivity, specific conductivity, cell constant. Mobility of ions, Conductometric titrations.

b) D.C Polarography :. Dropping mercury electrode- Instrumentation-polarogram. Types of Currents : Residual, Migration, Limiting. Two and Three electrode assemblies. Ilkovic equation (derivation not necessary) and its consequences. Types of limiting Currents : Adsorption, Diffusion, Kinetic. Applications of polarography in qualitative and quantitative analysis. Analysis of mixtures. Application to inorganic and organic compounds. Determination of stability constants of complexes.

c) Brief account of following techniques and their advantages over conventional d.c.polargraphy.

(i) A.C.polarography (ii) Square-wave polarography (iii) Pulse polarography (iv) Differential pulse polarography

d) Amperometric titrations :Principle, Instrumentation. Types and applications of amperometric titrations. Determination of SO_4^{2-}, metal ions viz., Mg^{2+}, Zn^{2+}, Cu^{2+} and other substances.

e) Cyclic Voltammetry : Principle, instrumentation, reversible and irreversible cyclic voltammograms. Applications. Cyclic voltammetric study of insecticide parathion.

ASP 06: : NMR spectroscopy-II (^{1}H,^{19}F and ^{31}P NMR)

^{1}H,^{19}F,^{31}P and solid state NMR spectroscopy: First order and non first order spectra e.g.,AX,AX_2,AX_3, A_2X_3,AMX and AB,ABC, Simplification of complex spectra: increased field strength, deuterium exchange,Lanthanide shift reagents and double resonance techniques. Discrimination of enantiomers by use of chiral NMR solvents (CSAs), chiral lanthanide shift reagents and Mosher's acid. Nuclear Overhauser enhancement (NOE).

Fluxional molecules- bullvalene, [η^5-C_5H_5M], [η^5-$(C_5H_5)_2$ Ti η^1-$(C_5H_5)_2$] and [$\eta^4C_8H_8Ru(CO)_3$].

^{19}F NMR spectroscopy: ^{19}F chemical shifts, coupling constants. Applications of ^{19}F NMR involving coupling with ^{19}F,^{1}H and ^{31}P: 1,2 dichloro-1,1 difluoro ethane, BrF_5, SF_4, PF_5, ClF_3, IF_5, HF_2^-.

^{31}P NMR spectroscopy: ^{31}P chemical shifts, coupling constants. Applications of ^{31}P NMR involving coupling with ^{31}P , ^{19}F, ^{1}H and ^{13}C: ATP, Ph_3PSe, P_4S_3, $P(OCH_3)_3$, H_3PO_4, H_3PO_3, H_3PO_2, HPF_2, PF_6^-, PH_3,[Rh $(PPh_3)Cl_3$] Rh I=1/2

Introduction to solid state NMR: Magic angle spinning (MAS).Applications of solid state NMR.

ASP 07: Mass spectrometry

Origin of mass spectrum, principles of EI mass spectrometer. Types of fragments: odd electron and even electron containing neutral and charged species (even electron rule), Nitrogen rule, isotopic peaks, determination of molecular formula, metastable ion peaks. High resolution mass spectrometry. Salient features of fragmentation pattern of organic compounds including β-cleavage, Mclafferty rearrangement, retro Diels – Alder fragmentation and ortho effect. Principle of EI, CI, Fast Atom Bombardment (FAB), Secondary Ion Mass Spectrometry (SIMS), Electrospray (ESI) ionization and Matrix Assisted Laser Desorption Ionization (MALDI) methods. Introduction to principle and applications of Gas Chromatography-Mass Spectrometry (GC-MS) and Liquid chromatography-Mass Spectrometry (LC-MS) techniques.

ASP-08: Photoelectron & ESR sprectroscopy

Photoelectron Spectroscopy

Principle and Instrumentation, Types of Photoelectron Spectroscopy – UPS & XPS
Binding Energies, Koopman's Theorem, Chemical Shifts.
Photoelectron Spectra of Simple Molecules: N_2, O_2, F_2, , CO, HF, NH_3 and H_2O - Vibrational Structure of PES Bands, Potential energy curves, Interpretation of Vibrational spectral data for ionized (M^+) species, Prediction of Nature of Molecular Orbitals. ESCA in qualitative analysis, Principles of Auger electron spectroscopy.

Electron Spin Resonance

Introduction, principle, instrumentation, selection rules, interpretation of Lande's factor 'g'. Hyperfine and super hyperfine Coupling. Anisotropy in 'g' values and hyperfine coupling constants. Zero field splitting, Kramer's degeneracy, quadrupolar interactions.
Study of free radicals and transition metal complexes. Evidence for covalency in complexes, ex. Cu(II) Bissalcylaldimine, Bis-acetylacetanatovanadyl(II) and hexachloroiridium(IV) complexes.

References:

1. Spectroscopic identification of organic compounds by R.M. Silverstein and F.X. Webster.
2. Organic spectroscopy by William Kemp
3. Mass Spectrometry for Chemists and biochemists by M. Rose and R.A. W. Johnstone
4. Spectroscopic methods in organic chemistry by D.H. Williams and I. Fleming
5. Practical Pharmaceutical Chemistry by A. H. Beckett and J.B. Stenlake
6. Biological Mass Spectrometry by A.L. Burlingame
7. Principles and Practice of Biological Mass Spectrometry by Chhabil Das
8. Spectrscopic identification of organic compounds by R.M.Silverstein. G.C.Bassler and T.E.Morrill
9. NMR-A multinuclear introduction by William Kemp
10. Stereochemistry of Carbon compounds by Ernest L Eliel / Samuel H. Wilen
11. Principles of Polarography, Heyrovsky.
12. Principles of Polarography, Kapoor.
13. Modern Electroanalytical methods, edited by C.Charlot, Elsevier Company.
14. Principles of Instyrumental analysis, Skoog, Holler and Nieman, Harcourt Asia PTE Ltd.
15. Analytical Chemistry-An Introduction, Skoog, West, Holler and Crouch, Saunders College Publishing.
16. Prinicples of Instrumental Analysis, Skoog and Leary, Saunders College Publishing.
17. International series of Monographs, Vol. **53**: Photoelectron Spectroscopy, Edited by D. Beckerand D. Betteridge 1972.
18. Sructural methods in inorganic chemistry, E.A.V. Ebsworth.

Paper CH 251P : Inorganic chemistry practicals: 6 hrs/ week

I. One component gravimetric estimations. (Use of sintered glass crucible)

(i). Estimation of Zn^{2+}.
(ii). Estimation of Ba^{2+}.

II. Analysis of Two component mixtures:

(i). Separation of Ni^{2+} and Cu^{2+} in a mixture and estimation of Ni^{2+} (gravimetric) and Cu^{2+} (volumetric).
(ii). Separation of Ag^{+} and Ca^{2+} in a mixture and estimation of Ag^{+} (gravimetric) and Ca^{2+} (volumetric).
(iii). Separation of Al^{3+} and Fe^{3+} in a mixture and estimation of Al^{3+} (gravimetric) and Fe^{3+} (volumetric).

III. Analysis of three component mixtures:

(i). Separation of (Fe^{2+} and Ni^{2+}) from Zinc (Zn^{2+}) in the given mixture and estimation of

Zinc (Gravimetric).

(ii). Separation of (Ni^{2+} and Cu^{2+}) from Mg^{2+} in the given mixture and estimation of Mg^{2+} (Gravimetric).

IV. Ion exchange methods of analysis:

(i). Determination of capacity of an ion exchange resin.

(ii). Separation of Zinc and Magnesium on an anion exchange resin and estimation of Mg^{2+} and Zn^{2+}.

Suggested Books :

1. Text book of Quantitative Inorganic Analysis by A.I.Vogel, 3rd edition, ELBS 1969.

2. Vogel's text book of Quantitative Inorganic analysis. Jeffery etal, 4th edition, ELBS 1988.
3. Vogel's text book of Quantitative Inorganic Analysis. 6 th edition, Pearson education Ltd. 2002.
4. Practical Inorganic chemistry By G.Marr and R.W.Rockett 1972.
5. Experimental Inorganic/Physical Chemistry – An Investigative integrated approach to Practical Project work. By Mounir A.Malati, 1999.
6. Advanced experimental Inorganic chemistry by. Ayodhya Singh.
7. Practical Inorganic Chemistry by G.Pass & H. Sutchiffe, 2nd edn John Wiley &Sons.

Paper CH 252P : Organic Chemistry Lab: 6 hrs / week

Identification of organic compounds, systematic qualitative analysis:

Physical data BP / MP, Ignition test, Lassaigne test – Nitrogen, Sulphur and halogens, solubility classification

Functional groups tests, Preparation of crystalline derivative and determination of their m.p.s and reference to literature to identify the compounds

A minimum of **14** compounds covering different functional groups and solubility pattern. Glucose, benzoic acid, 2-chloro benzoic acid, anisic acid, p-nitrobenzoic acid; p-cresol, p-chlorophenol, β-naphthol; aniline, o/m/p-chloroanilines; N-methylaniline/N-ethylaniline, N,N-dimethylaniline, benzamide, acetanilide, benzaldehyde, anisaldehyde, acetophenone, benzophenone, ethylbenzoate, methylbenzoate, nitrobenzene, chlorobenzene, bromobenzene , naphthalene, biphenyl and anthracene.

Identification of unknown organic compounds from their IR, UV, ^{1}H NMR and Mass Spectral data:

Analysis of recorded spectra of compounds belonging to i)alkynes, ii) alcohols and phenols iii) aldehydes and ketones iv)carboxylic acids,v) esters vi) acid amides and vii) primary and secondary amines.

References

1. Text book of practical organic chemistry, Vogel
2. Text book of practical organic chemistry, Mann and Saunders.
3. Spectral identification of organic compounds Bassler, Silverstein 5th Edition

Paper CH 253P : Physical Chemistry Lab: 6 hrs /week

Distribution:

1) Distribution of I_2 between CCl_4 and aq.KI solution- calculation of equilibrium constant.
2) Study of complex formation between ammonia and metal ion

Chemical Kinetics

1) Stoichiometry of peroxydisulphide- iodide reaction
2) Peroxydisulphide- iodide reaction: order w.r.t [I-] by isolation method
3) Peroxydisulphide- iodide reaction: order w.r.t $[S_2O_8^{2-}]$ by initial rate method

Condutometry:

1) Titration of a mixture of strong and weak acids vs strong base
2) Determination of the hydrolysis constant of aniline hydrochloride
3) Determination of solubility product

Potentiometry:

1)Titration of Fe^{+2} vs $Cr_2O_7^{-2}$ (redox titration)
2)Titration of Cl^- vs Ag+ (precipitation titration)
3)Determination of solubility product

Polarimetry:

1)Determination of specific rotation of glucose and fructose
2)Enzyme catalysed inversion of sucrose

Colorimetry:

1)Verification of Beer's law and calculation of molar absorption coefficient using $CuSO_4$ and $KMnO_4$ solutions

pH metry:

1)Calibration of a pH meter and measurement of pH of different solutions
2)Preparation of phosphate buffers

Solutions:

1)Determination of molecular weight of a non volatile substance by cryoscopic method
2)Determination of degree of dissociation by cryoscopic method
3)Study of surface tension-concentration relationship for solutions (Gibbs equation)

INORGANIC CHEMISTRY SPECIALISATION

SYLLABUS (2012 – 13) ONWARDS

M.Sc. CHEMISTRY(ORGANIC CHEMISTRY)

III & IV SEMESTERS

FOR STUDENTS ADMITTED IN THE YEAR (2011 – 12)

REVISED AS PER NEW (CB) SYLLABUS

M.Sc.CHEMISTRY(INORGANIC CHEMISTRY)

Syllabus for III and IV Semesters

(For the batch admitted during the academic year 2011-2012 under the CBCS pattern)

[Under Restructured CBCS Scheme]

(Approved in the P.G. BOS meeting held on 15-9-2012)

Semester - III

	Instruction	Internal assessment	Semester exam*	Total	Credits
	Hrs/week	**marks**	**marks**	**marks**	
CH(IC) 301T	4	20	80	100	4
CH(IC) 302T	4	20	80	100	4
CH(IC) 303T	4	20	80	100	4
CH(IC) 304T	4	20	80	100	4
SEMINAR	2	--	--	25	1
CH(IC) 351P	9	--	100	100	4
CH(IC) 352P	9	--	100	100	4
Total				**625**	**25**

*Theory: 3 hours; Practical's: 6 hours

Semester - IV

	Instruction	Internal assessment	Semester exam*	Total	Credits
	Hrs/week	**marks**	**marks**	**marks**	
CH(IC) 401T	4	20	80	100	4
CH(IC) 402T	4	20	80	100	4
CH(IC) 403T	4	20	80	100	4
CH(IC)404T (CB)	4	20	80	100	4
SEMINAR	2	--	--	25	1
CH(IC) 451P	9	--	100	100	4
CH(IC) 452P	9	--	100	100	4
Total				**625**	**25**

(**Choice based paper (CB) =** Paper offered by the same Department or other Department in the Science faculty)

*Theory: 3 hours; Practical's: 6 hours

Grand total (all 4 semesters), 2500 marks and 100 credits

PAPER TITLES

M.Sc. INORGANIC CHEMISTRY SPECIALISATION

III SEMESTER SYLLABUS

(For the batch admitted during the academic year 2011-2012 under the CBCS pattern)

[Under Restructured CBCS Scheme]

SEMESTER--III

PAPER-1 :CH(IC)301 T: Bonding, Group Theory and its Applications

IC-09: Group Theory, Normal mode analysis and Spectral Activity

IC-10: MOT of Metal Complexes

IC-11: Electronic Spectroscopy of Metal Complexes

IC-12: IR and Raman Spectroscopy

CH(IC) 302T : Molecular Spectroscopy of Inorganic Compounds

IC-13: Multinuclear NMR

IC-14: Advanced NMR techniques

IC-15 Applications of ESR to Metal Complexes

IC-16 : Mossbauer Specroscopy and Nuclear Quadrupole Resonance Spectroscopy

CH(IC)303T : Organo metallic Chemistry of Transition Metal Complexes

IC-17: Mono,Di and Tri hapto Complexes

IC-18: Tetra,Penta,Hexa,Hepta and Octa hapto Complexes

IC-19: Catalytic Role of OTMC-I

IC-20: Catalytic Role of OTMC-II

CH(IC) 304 T: Photochemistry, Thermal , Diffraction and Mass spectrometry Methods

IC-21: Photochemistry of Metal Complexes

IC-22: Thermal Methods, AAS, AES, ICP-AES

IC-23:, Diffraction Methods

IC-24: Advanced Mass spectrometry & Hyphenated Techniques

LABORATORY COURSES

PAPER-V CH (IC) 351P: Synthesis and Characterization of Metal Complexes

PAPER–VI CH (IC) 352 P: Electro-analytical techniques

PAPER TITLES

M.Sc. INORGANIC CHEMISTRY SPECIALISATION

IV SEMESTER SYLLABUS

(For the batch admitted during the academic year 2011-2012 under the CBCS pattern)

[Under Restructured CBCS Scheme]

SEMESTER-IV

PAPER-I :CH(IC) 401T: Inorganic Biochemistry

IC-25: Metal ions Interactions with Nucleic acids and their constituents.
IC-26: Transport of Electrons and Metal ions.
IC-27: Metallo-Enzymes of Iron,Zinc and Nickel.
IC-28: Metallo-Enzymes of Cobalt,Copper and Molybdenum.

CH (IC) 402T: Medicinal Inorganic Chemistry

IC-29: Metal complexes as Drugs and Anticancer agents
IC-30: Metal complexes in Clinical Chemistry
IC-31: Chemical and Photochemical probing of DNA complexes
IC-32: DNA binding and molecular pharmacology and Interaction of Metallo Pharmaceuticals

CH(IC) 403T: Supra Molecular Chemistry and Bio Physical Studies

IC-33: Supramolecular Chemistry

IC-34: Structural aspects of DNA and RNA
IC-35: Spectroscopic analysis of drug/metal complexes binding to Nucleic acid:
IC-36: CD ,ORD, Fluorescence and Enzyme kinetics

CH(IC) 404(CB_1)T: Separation Methods, Data Handling, Green Chemistry and Nanotechnology

IC (CB_1)-1: Separation Methods
IC (CB_1)-2: Data Handling
IC (CB_1)-3: Green Chemistry
IC (CB_1)-4: Nanotechnology

CH(IC) 404 (CB_2) T : Applied Analysis

IC (CB_2)-1: Data Handling
IC (CB_2)-2: Analysis of Air and Water Pollutants
IC (CB_2)-3: Clinical and Pharmaceutical analysis
IC (CB_2)-4: Food and Agricultural analysis

LABORATORY COURSES

PAPERV CH (IC) 451P: Spectroscopic techniques

PAPERVI CH (IC) 452P: Structural Assignment of Metal Complexes from Physico-Chemical Data &ConventionaLMethods of Analysis

M.Sc. INORGANIC CHEMISTRY SPECIALIZATION
Syllabus for III and IV Semesters
(For the batch admitted during the academic year 2011-2012 under the CBCS pattern)
[Under Restructured CBCS Scheme]

SEMESTER-III

PAPER I

CH(IC)301T: Bonding, Group Theory and its Applications

IC-09: Group Theory, Normal mode analysis and Spectral Activity

IC-10: MOT of Metal Complexes

IC-11: Electronic Spectroscopy of Metal Complexes

IC-12: IR and Raman Spectroscopy

IC-09: Group Theory, Normal Mode Analysis and Spectral Activity

Properties of a Group-Closure rule, Identity rule, associative rule, inverse rule, Abelian and Non-abelian groups. Classes of Symmetry Elements of a Group: Similarity transformation, properties of conjugate elements, rules of Classes, Classes of C_{2V}, C_{2h} and C_{3V}. Matrix Representation of Symmetry Elements: Simple Matrices, Matrix addition, subtraction and multiplication, Block-Factorization. Matrix Representation of *E*, C_n, S_n, i and σ Elements and C_{2V}, C_{3V}, C_{2h}, C_{4V} & D_{2h}.Great Orhogonality Theorem: Reducible and Irreducible Representations, Properties of Irreducible Representations, Construction of Character Tables for C_{2V}, C_{2h} and C_{3V}. Mulliken Symbolism for Irreducible Representations - Standard Reduction Formula – Direct Products.

Use of Character tables for IR & Raman spectroscopy, symmetry based selection rules for for IR and Raman activity. Standard reduction formula. Type and Symmetry of Normal Modes and IR and Raman activity of molecules: Cartesian coordinate method of analysis for C_{2V} (eg H_2O/SO_2, SF_4, ClF_3, Cis-N_2F_2), C_3V ($NH_3/SO_3^{2-}/PCl_3$, $POCl_3$), C_{2h} (trans-N_2F_2), D_{3h} (CO_3^{2-}/BF_3), Td($SO_4^{2-}/PO_4^{3-}/ClO_4^-/NH_4^+$), Oh ($SF_6$). Internal coordinate method of analysis for C_{2V} (H_2O), C_3V (NH_3), Td (SO_4^{2-}). Internal Coordinates and Redundancy (Qualitative concept).

IC-10: Molecular Orbital Theory of Metal Complexes

Symmetry Classification of Metal and Ligand Orbitals in Cubic and Non-Cubic Environments: Octahedral, Tetrahedral, Square Planar, Square Pyramidal, Trigonal Bipyramidal Geometries – Concept of Ligand Group Orbitals – Construction of Molecular Orbital Energy Level Diagrams for Octahedral, Tetrahedral and Square Planar Metal Complexes with Sigma (σ) and Pi (π) Bonding Contribution from the Ligands.

IC-11: Electronic Spectroscopy of Metal Complexes

Classification of Electronic Spectra for Metal Complexes, Selection Rules: Electric Dipole Transitions, Magnetic Dipole Transitions, Orbital Selection Rules, Spin Selection Rules, Relaxation in Selection Rules. Nature of Electronic Spectral Bands: Band Widths, Band Intensities. Factors Influencing Band Shapes: Jahn-Teller Effect, Spectrochemical Series, Nephelauxetic Effect. Orgel Diagrams for d^1-d^9 Configurations, Crystal Field Spectra of O_h and T_d Metal Complexes of 3d Metals. Charge Transfer Spectra. Strong Field Configurations: The Method of Descending Symmetry, Correlation Diagrams and Tanabe-Sugano Diagrams for d^2 and d^8 Configurations. Calculation of 10Dq Values, Racah Parameter (B) and Nephelauxetic Ratio (β) .

IC-12: Infrared and Raman Spectroscopy

Conditions for Infrared and Raman Spectroscopies – Structure Fitting. Determination of Coordination Sites and Linkage Isomers(NO_2^- , SCN^-), Assigning Denticity of Ligands (SO_4^{2-}, CO_3^{2-}), Prediction of Diagnostic Fundamentals in Isomers of Metal Complexes and Distinguishing Isomers of Metal Complexes. Effect of Coordination on Ligand Vibrations: Examples involving Mono, Bi and/or Polydentate Ligands of Oxygen, Sulfur, Nitrogen, Phosphorous, Carbon and Halogen Donors (NH_3, H_2O, Glycine, PPh_3, 2,2,-Bipy, 1,10-Phen, Carbonyl and halides). Raman effect and molecular structure- CO, HCN, CO_2, N_2O, H_2O. Principles of Resonance Raman Spectroscopy.Application of Resonance Raman Spectroscopy to Structural Elucidation of the active Sites of Heme and Non-Heme Oxygen Carriers.

SUGGESTED BOOKS

1. *Symmetry and Spectroscopy of Molecules*, K. Veera Reddy, Second Edition, New Age International (P) Limited Publishers (2009)
2. *Chemical Applications of Group Theory,* F. A. Cotton, 3rd edition, Wiley NY (1990)
3. *Symmetry and Group Theory In Chemistry*, Mark Ladd, Harwood Publishers, London (2000)
4. *Symmetry Through the Eyes of a Chemist,* I. Hargittai and M. Hargittai, 2nd Edition, Plenum Press, NY (1995)
5. *Molecular Symmetry and Group Theory,* Robert L. Carter, John Wiley & Sons (1998)
6. *Group Theory for Chemists,* G. Davidson, Macmillan Physical Science Series (1991)
7. *Molecular Symmetry,* Schoenland
8. *Electronic Spectroscopy,* A. B. P. Lever
9. *Introduction to Ligand fields,* B. N. Figgis
10. *Infrared and Raman Spectroscopy of Inorganic and Coordination Compounds,* K. Nakamoto
11. *Infrared spectroscopy of Inorganic Compound,* Bellamy.

Paper II

CH(IC) 302T : Molecular Spectroscopy of Inorganic Compounds

IC-13: Multinuclear NMR
IC-14: Advanced NMR techniques
IC-15 Applications of ESR to Metal Complexes
IC-16 : Mossbauer Specroscopy and Nuclear Quadrupole Resonance Spectroscopy

IC-13 Multinuclear NMR

^{13}C nmr spectroscopy: CW and PFT techniques. Types of ^{13}C nmr spectra: undecoupled, proton- decoupled, single frequency off-resonance decoupled (SFORD) and selectively decoupled spectra. ^{13}C chemical shifts, factors affecting the chemical shifts.

Chemical equivalence and magnetic equivalence. Virtual Coupling and its importance in study of Metal Complexes $[Pd\{P(CH_3)_3\}_2I_2]$. Spin Dilute Systems-Satellites in Pt(II) Complexes cis-$[Pt(PEt_3)_2Cl_2]$, $Sn(CH_3)_4$. NMR Time Scale and its use in studying Stereo chemical Non –rigidity (PF_5, $[Rh(PR_3)_5]^+$, $[Fe\{Cp\}_2(CO)_2]$) -ΔR, the Ring Contribution to ^{31}P Chemical Shifts –Metal and Chelate size on ΔR. Applications of ^1H, ^{13}C, ^{19}F, ^{31}P and ^{15}N to simple inorganic and Coordination Compounds - 1)^1H-NMR: $PtHCl(PEt_3)_2$, $Pt(NH_3)_3(CH_3)_3$, BH_4^-, NH_4^+, CH_3CN, [^{6}h- C_7H_8 $Mo(CO)_3$], [^{7}h-$C_7H_7Mo(CO)_3]^+$, B_2H_6; $^{29}SiH_3SiH_3$, 2)^{19}F: BF_4^-, H_2PF_3 3)^{31}P: $Mo(CO)_3(PPh_3)_3$, [Rh $(PPh_3)_3Cl$] ,trans-$[PtCl_4(PEt_3)_2]$, $^{31}PF_2H(^{15}NH_2)_2$ 4) 13C; [^{4}h C_8H_8 $Ru(CO)_3$], $Fe(CO)_5$, $Fe_2(CO)_9$, $Fe_3(CO)_{12}$, $FeICp(CO)_{12}$, [$^{13}C^{15}N$ $Co(DH)_2$Pyridine]. $^{13}C\{^1H\}$ NMR spectrum of σ-bonded C_6H_5 ligand.

IC-14 Advanced NMR Spectroscopy: - Spin-Lattice (T_1) and Spin-Spin Relaxation (T_2). Spin Echo Polarization Transfer – Spin Echo Measurements. ^{13}C-NMR spectral editing techniques: Attached proton test (APT spectra) by Gated Spin Echo, Cross polarization, INEPT spectra, DEPT spectra (Distortionless enhancement by polarization transfer) (eg $Cl(CH_2)_3Si(OCH_3)_3$). INADEQUATE spectra (Incredible Natural Abundance Double Quantum Transfer Experiment).

Two Dimensional NMR: Basic principles, Types of 2-D NMR ;i)J- resolved spectroscopy a)homo and b)Heteronuclear J- resolved spectroscopy ii) Correlation spectroscopy ; Homo nuclear shift correlation spectroscopy (COSY) and Hetero nuclear shift correlation spectroscopy (HETCOR) iii) NOESY(Nuclear Overhauser Enhancement Spectroscopy). HOESY (two dimensional heteronuclear NOE). Advantages of 2-D NMR

IC-15: Applications of ESR to Metal Complexes

Principle- Selection Rules – Instrumentation- Microwave source(energy bands). Application of ESR to the study of simple free radicals: methyl ($CH_3^{\cdot}$), amine ($NH_2\cdot$), diphenylpicryl hydrazyl, cyclopentadienyl ($C5H5^{\cdot}$), hydroxy methyl ($CH2OH\cdot$) radicals. Zero-Field Splitting (ZFS) - Effective Spin - Orbitally Non-degenerate and Degenerate States. ESR Spectra of d^1-d^9 Transition Metal Complexes with examples. Interpretation of g in cubic, axial and rhombohedral geometries. Factors affecting g values. Calculation of g values with

simple examples. Intensities of '$g_{\parallel}$ and g $\perp$ peaks . Evidence for Metal-Ligand Bond Covalency- Cu(II)- Bis –Salicylaldimine. $[(NH_3)_5\,Co\,O_2\,Co\,(NH_3)_5]^{5+}$, Cu(II)- diethyldithio phosphinate, Vanadyl dithio phsphinate, Copper(II) tetraphenyl porphyrin, Co(II)-phthalocyanine, $K_2[IrCl_6]$. Interpretation of 'g' and 'A' values from esr spectral data in- i) MnF_6^{4-}, ii) CoF_6^{4-}, and CrF_6^{3-}. ESR spectra of dinuclear Cu (II) complexes.

IC-16 Mossbauer and Nuclear Quadrupole Resonance Spectroscopy

Mossbauer Spectroscopy Principle, Experimental Considerations and Presentation of the Spectrum - Isomer Shifts – Quadrupole splitting and Magnetic hyperfine splitting - Selection Rules.

Applications

Iron Compounds: Low-spin and High-spin Fe(II) and Fe(III) Complexes - π-bonding Effects in Iron complexes - Study of High-spin Low-spin Cross-over c) Diamagnetic and Covalent Compounds - Structural aspects of Iron Carbonyls and Iron-Sulfur Proteins

Tin Compounds: Tin Halides and Organotin Compounds.

Iodine Compounds: Isomer Shifts of ^{127}I and ^{129}I - Applications to Alkali metal iodides and Molecular Iodine. .

Nuclear Quadrupole Resonance Spectroscopy : Principle, nuclear quadrupole resonance experiment, structural information from NQR spectra, Interpretation of nuclear quadrupole coupling constants.

SUGGESTED BOOKS

1. Structural Methods in Inorganic Chemistry, E. A. V. Ebsworth, D. W. H. Rankin and
2. S. Craddock, ELBS.
3. Physical Methods in Chemistry, R. S. Drago, W.B. Saunders Co., 1977.
5. Physical Methods for Chemists, Russell S. Drago Second edition, Saunders College Publishing, 1992.
6. Principles of Mossbauer spectroscopy, T. C. Gibb, Chapman and Hall, London, 1976.
7. Mossbauer Spectroscopy, N. N. Greenwood and T. C. Gibb, Chapman and Hall, London, 1971.
8. Principles of Instrumental Analysis, Skoog, Holler and Nieman.
9. Instrumental Techniques for Analytical Chemistry, Frank Settle.
10. Principles of Analytical Chemistry, M. Valcarcel.
11. Physical Methods in Advanced Inorganic Chemistry, Hill and Day
12. Magneto Chemistry, Dutta & Shyamal Oxford Chemistry Primers, Vol 62

PAPER III

CH(IC)303 T: Organo metallic Chemistry of Transition Metal Complexes

IC-17: Mono,Di and Tri hapto Complexes
IC-18: Tetra,Penta,Hexa,Hepta and Octa hapto Complexes
IC-19: Catalytic Role of OTMC-I
IC-20: Catalytic Role of OTMC-II

IC-17: Mono, Di and Tri hapto Complexes

Nomenclature and Classification based on the number of Coordinated Carbons (hapticity) and number of electrons donated by the Ligand. η1 – Complexes : General methods of Preparation –Bonding of Ligand to Metal :α and β Interaction – Thermodynamic Stability and Kinetic Lability of η1 Complexes –Tertiary Phosphine – Transition Metal Alkyl and Aryl Complexes of Ni, Pd and Pt – Ortho-effect – Bonding in Metal – Carbene and Carbyne Complexes. η2 –Complexes : General methods of preparation of Metal – Alkene Complexes – Structure and Bonding in η2 Complexes – Factors affecting the stability of Metal-Olefin bond – Trans Effect – Rotation of Olefin around Metal-Olefin Bond. η3 - Complexes : Metal-Allyl Complexes – General Preparative Routes – Structure and Bonding in η3 Allyl Complexes – Fluxionality –Reactions of η3 Allyl Complexes.

IC-18: Tetra, Penta,Hexa,Hepta and Octa hapto Complexes

η4 Complexes : Structure and Bonding in η4 Complexes –Butadiene and Cyclobutadiene Complexes and their Reactivity. η5 – Complexes : Classification and General methods of Preparation – Bis (η5-cyclopentadienyl) metal complexes (Metallocenes) – Ferrocene : Structure and Bonding –Reactions of Ferrocene – Mechanism of Electroplilic substitution – Friedel Crafts acylation, alkylation, nitration, halogenation and Metallation Reactions.
η6 Complexes : Metal –Arene Complexes – Dibenzenechromium – Preparation, Structure and Bonding in Bis(arene)-Metal Complexes – Reactions. η7 Complexes : Preparation , Structure and Reactions of η7 – C_7H_7 Complexes. η8 Complexes : C_8H_8 as a Ligand – Cyclooctatetraene Complexes – Preparation, Structure and Bonding in Uranocene.

IC-19: Catalytic Role of OTMC-I

Oxidative addition and Reductive Elimination : Stereochemistry and Mechanism of Oxidative Addition – Insertion Reactions – Hydrogenation of Olefins –Transfer Hydrogenation – Hydrosilation of Olefins – Isomerisation of Olefins – Ziegler –Natta Polymerization of Olefins – Oligomerization of Butadiene Alkene Metathesis. Dupont-1,4-hexadiene synthesis.Oxidation of Olefins to Carbonyl Compounds – Oxidation of Hydrocarbons to Alcohols and Acids – Oxidation of Aldehydes, Cyclohexanol, Cyclohexanone, p-Xylene.

IC-20: Catalytic Role of OTMC- II

Reactions of Carbon monoxide and Hydrogen : Hydroformylation – Carbonylation –Syngas-Water gas shift Reaction (WGS) – Reactions of Syngas. Applications of Metal Clusters in Catalysis : Hydroformylation of Ethylene using $[HRu_3(CO)_{11}]$ – , Hydrogenation of Olefins. Use of $[Fe_4C(CO)14]$ as a model for Fischer – Tropsch process. Recent Developments in Homogenous Catalysis: Phase Transfer Catalysis (PTC) – Homogeneous Transition Metal Catalyzed Reactions under Phase Transfer Conditions: Hydrogenation. Bio Catalysis : Enzyme Analogue Catalysis: Introduction, Examples of Enzymatic Conversions, Reduction of >C=O and >C=C< bonds, Templates: Introduction, Metal Cations as Templates, Covalent molecules as Templates, External and Internal Templates – Homogeneous Catalysts and their

Heterogenization or Immobilization by Aqueous Catalysis.

SUGGESTED BOOKS

1.*Organometallics*-A Concise Introduction, Ch.Eischeinbroich and Salzer-VCH
2.*Organotransition Metal Chemistry Fundamental Concepts and Applications*, John Akio Yamamato, Wiley & Sons.
3.Homogeneous Catalysis by Metal Complexes, M M Taqui Khan and A E Martel
4. Applied Homogenous Catalysis with Organo Metallic Compounds Vol I & II, Boy Cornills and W A Herrmann – VCH
5. Organometallic Compounds, G E Coates, M C H Green, K Wade vol II
6. Advanced Inorganic Chemistry, Cotton and Wilkinson, V & VI Ed
7. Symmetry and spectroscopy, K Veera Reddy
8. Homogenous catalysis, G W Parshall, John Wiley & Sons, New York

PAPER- IV

CH(IC) 304T: Photochemistry, Thermal , Diffraction and Mass spectrometry Methods

IC-21: Photochemistry of Metal Complexes
IC-22: Thermal Methods, AAS, AES, ICP-AES
IC-23:, Diffraction Methods
IC-24: Advanced Mass spectrometry & Hyphenated Techniques

IC-21: Photo Chemistry of Metal Complexes

Energy, Structure, Electron Distribution and Chemical reactivity of Electronically Excited states of Coordination Compounds. Photochemistry of Cr(III) and Co(III) metal complexes . Photochemistry of Cr(CO)6 ,$Mn_2(CO)_{10}$ and $Fe(CO)_5$.

Sharp line phosphorescence of Ruthenium Bipyridyl and Ortho-phenanthroline Complexes. Energy transfer Spin Correlation energy levels in the energy Transfer Systems;$[Ru(bipy)_3]^{2+}$ $[Cr(CN)_6]^{3-}$. Metal Sensitizers and Quenchers - Electron Relay. Photochemical Hydrogen production by oxidative quenching of $[Ru(bipy)_3]^{2+}$* by Methyl Viologen.

IC-22: Thermal Methods, AAS, AES, ICP-AES

Thermal methods of analysis: Thermogravimetry, Differential Thermal Analysis and Differential Scanning Calorimetry, instrumentation. Methodology of TG, DTA and DSC. Applications: study of oxalates and chromates. Determination of Glass transition, Heat capacity determination, Characterization of polymer blends.

Atomic Absorption Spectroscopy (AAS): Principles of AAS, Instrumentation – flame AAS and furnace AAS, resonance line sources, sensitivity and detection limits in AAS, interferences –chemical and spectral, evaluation methods in AAS and application in qualitative and quantitative analysis.

Atomic Emission Spectroscopy (AES): Principles of AES, Instrumentation, evaluation methods, Application in quantitative analysis.

Inductively Coupled Plasma - Atomic Emission Spectroscopy (ICP-AES): Limitations of AES, Principles of plasma spectroscopy, plasma as an excitation source. Inductively coupled plasma source, ICP-AES – Instrumentation. Application of ICP-AES, Comparison with AAS.

IC-23:, Diffraction Methods

X – ray Diffraction : X –rays and their generation – choice of radiation ; Miller indices, Braggs equation, Experimental methods – Powder and single crystal methods, Indexing the reflections, Systematic absences, Electron density studies by X – rays – Platinum phthalocyanine complex, Silyl acetate, Tetraalkyl biphosphate ; Advantages and limitations of X – ray Diffraction.

Electron Diffraction by gases :__Principles , Radial distribution curves- Interpretation of results for $PBrF_2S$, PF_3S, PF_2HS, $HClO_4$, Silyl monothioacetate and Germyl monothioacetate and HgCl2 molecules, Advantages and Limitations

Neutron Diffraction: Principle, Application in Hydrogen bonding studies, combined use of X – ray and Neutron diffraction studies , Advantages and limitations.

IC-24: Advanced Mass spectrometry & Hyphenated Techniques

Advanced Mass spectrometry

Quadruple analysers, Ion traps. Time of flight mass spectrometry.

Quantitative mass spectrometry: Introduction and Principles; Calibration and Internal Standards; Selected ion monitoring – Selecting ions for monitoring.

Mass Spectrometry / Mass Spectrometry : Tandem Mass Spectrometry. Ion cyclotron resonance spectrometers and Ion traps for MS/MS.

Hyphenated Techniques: GC-MS Principle, instrumentation, Interfaces- Direct coupling interface and open split interface. Application based on gas chromatography/mass spectrometry-Analysis of metabolite of drug Imipramine. **LC-MS-** principle, Instrumentation – Interfaces- Moving belt interface, particle beam interface, thermospray interface, Electrospray interface, atmospheric pressure chemical ionization interface. **ICP – MS** - Principle and Instrumentation,

SUGGESTED BOOKS

1. Concepts of Inorganic PhotoChemistry A.W. Adamson and P. D. Fleschaner,Wiley.
2. Inorganic Photochemistry, Journal of Chemical Education, Vol 60. No 10, 1983.
3. Progress in Inorganic Chemistry Vol 30 ed :S.J.Lippard.
4. Coordination Chemistry Reviews Vol 39 1981,p121
5. Photochemistry of Coordination compounds V.Balzani and Carassiti,academic presss.
6. Elements of inorganic Photochemistry G.J.Ferrendi,Wiley,
7. Structure and Bonding Vol 49 1982.
8. Principles of Instrumental Analysis, Skoog, Holler and Nieman.
9 . Instrumental Techniques for Analytical Chemistry, Frank Settle.
10. Principles of Analytical Chemistry, M. Valcarcel.
11. Solid State Chemistry and its Applications, *West.*
12. Introduction to Solids, Azaroff.
13. Solid State Chemistry, D.K. Chakrabarthy
14. Physical Methods in Advanced Inorganic Chemistry, Hill and Day.
15. Instrunmental Methods of Analysis, Sixth edition, CBS Publishers, Willard, Merrit, Dean, and Settle.
16. Mass spectrometry for Chemists and Biochemists, Robert A.W Johnstone and Molcolm. E.Rose second Edn.
17. Physical methods for Chemists, Russell S. Drago second edition, Saunders College publishing 1992.
18. Structural methods in Inorganic Chemistry, E.A.V. Ebsworth, D.W.H Rankin and S. Craddeck, ELBS.
19. Mass spectrometry Basics Johnstone

SEMESTER-III

LABORATORY COURSES

Paper CH (IC) 351P: Synthesis and Characterization of Metal Complexes

preparation and characterization of *3d* transition metal complexes of *tetrahedral square planar* and *octahedral* geometries.

1. $Mn(acac)_3$
2. $VO(acac)_2$
3. $Ni(DMG)_2$4.
4. $CoCl_2\ (Py)_2$

5. $[Co(NH_3)_6][Co(NO_2)_6]$
6. *Cis*-$[Co(trien)(NO_2)_2]Cl.H_2O$
7. $Na[Cr(NH_3)_2(SCN)_4]$
8. $TiO(C_9H_6NO)_2.2H_2O$

9. Prussian Blue, Turnbull's Blue Complexes

SUGGESTED BOOKS

1. *Practical Inorganic Chemistry*, G. Marr and B. W. Rockett.
2. Practical Inorganic Chemistry by G.Pass H.Sutchiffe,2nd edn John Wiley & Sons.
3. *Experimental Inorganic/Physical Chemistry,* M. A. Malati, Horwood Publishing, Chichester, UK (1999)

Paper CH (IC) 352: Electro-analytical techniques

I Potentiometry

Potentiometric Titrations and Calculation of End Point Potentials for the following systems:

i) Fe^{2+} vs $Cr_2O_7^{2-}$
ii) Fe^{2+} vs MnO_4^-
iii) $Fe^{2+}$and VO^{2+} Mixture vs Ce^{4+}
iv) Assay of sulphanilamide
v) Silver electrode for silver assay
vi) Mixture of halide anions using Silver electrode

II pH-metry

1. Determination of CO_3^{2-} and HCO_3^- in a mixture
2. Determination of the dissociation constants of

(i) Ethylenediamine (en)(H_2 L) (ii) Glycine (HL) (iii) Histidinemonohydrochloride (H_2L)

3. Determination of binary constants of i) Cu(II) -en and (ii) Ni(II) -His iii) Ni(II) – Gly Systems
4. Determination of stability constant of ternary (o-Phen-Ni(II)-His) system - Calculation of Log K.

III Conductometry:

1. Determination of the Composition of Cu(II)-oxine and Cu(II)-EDTA Complexes
2. Interaction of Pyrophosphate with Mg^{2+}, Ca^{2+}, Mn^{2+} and Cu^{2+}
3. Determination of Aspirin with KOH

IV Polarography

1. Determination of $E_{½}$ of Cd^{2+} and Pb^{2+}
2. Verification of Ilkovic equation by using Cd^{2+} solution
3. Determination of Stability Constants of Cd^{2+} and Pb^{2+} complexes

V Electrogravimetry

1. Determination of Copper and Nickel individually and in a Mixture

References:

1. A Text Book of Quantitative Inorganic Analysis by A.I.Vogel 3rd Edition Elbs Publication 1969.
2. Vogel's Text Book Of Quantitative Inorganic Analysis Jeffery etal 4th edition Elbs Publications 1988.
3. Vogel's Text Book of Quantitative Chemical Analysis, 6th edition. Pearson Education Ltd 2002.
4. Determination and use of Stability Constants – Martell and Motekaitis VCH Publishers INC 1988.
5. Metal Complexes in Aqueous Solutions A.E.Martell and R.D. Handcock, Plenum Press, New York – 1996.
6. Analytical Chemistry by Gary D.Christian 6th EditionJohn Wiley&Sons Inc New York 1994.

M.Sc. CHEMISTRY(INORGANIC CHEMISTRY)
IV SEMESTER SYLLABUS
PAPER I

CH(IC) 401T: Inorganic Biochemistry

IC-25: Metal ions Interactions with Nucleic acids and their constituents.
IC-26: Transport of Electrons and Metal ions.
IC-27: Metallo-Enzymes of Iron,Zinc and Nickel.
IC-28: Metallo-Enzymes of Cobalt,Copper and Molybdenum.

IC-25: Metal Ion Interactions with Nucleic Acids and their Constituents

Proton Binding Sites of Nucleic Acid Constituents: Purine and Pyrimidine Bases, Nucleosides and Nucleotides - General Factors that influence Metal Ion Binding Sites in Solution – Specific Metal Ion Binding to Nucleic Bases, Nucleotides and Nucleosides in Solution: Stability of Phosphate- Metal ion complexes, Metal binding Metal Ion Complexes, Metal Binding Sites in Nucleosides, Nucleotide - Metal Ion Interactions - Intramolecular Equilibrium Constant KI, Percentage of Closed Isomers - Outer Sphere and Inner Sphere Isomers of M-ATP Complexes and Metal Ion Nucleic Base Interactions.
Metal-DNA and RNA Interactions: Potential Binding Sites (Elementary Treatment) – Influence of Metal Ions on Stability of Nucleic Acids – Concept of TM.

IC-26:Transport of Electrons and Metal Ions

Transport of Electrons: Iron-Sulphur Proteins: Rubredoxins and Ferredoxins (2Fe, 3Fe, 4Fe, 8Fe Proteins) - High Potential Iron-Sulphur Proteins – Structural and Spectral features of Iron-Sulphur Proteins - Electron-transport by Cytochromes, Azurin and Plastocyanin - Importance of Structures of Azurin and Plastocyanin in facilitating Rapid Electron Transport.
Transport and Storage of Metal Ions: Iron-Transport by Transferrin and Siderophores – Ferritin in Iron Storage - Transport of Na+ and K+ across Cell Membranes by Na^{+}- K^{+} ATPase - Transport of Calcium across Sarcoplasmic Reticulam by Ca^{2+}-ATPase.

IC-27: Metallo-Enzymes of Iron, Zinc and Nickel

Iron Enzyme: Structural and Mechanistic Aspects of Cytochrome P450, Cytochrome oxidase, Catalase and Peroxidase - Role of the Metal Ion.
Zinc Enzymes: Structural and Mechanistic Aspects of Carbonic Anhydrase, Carboxy Peptidase,Alcohol Dehydrogenase - Role of Zinc.
Nickel Enzyme: Urease, Hydrogenase and Factor F430: Reactions Catalysed , Mechanistic Aspects.

IC-28: Metallo-Enzymes of Cobalt, Copper and Molybdenum

Cobalt Enzymes: Cobalt in Vitamin B12 - Structural Features of Vitamin B12 with reference to coordination of Cobalt - Different Oxidation States of Cobalt - Various forms of Vitamin B12 and Active Enzyme forms - Types of Reactions Catalysed by i) Methyl Cobalamin ii)Deoxyadenosyl Cobalamin - Mechanism of the Methyl Malonyl CoA conversion to Succinyl CoA - Role of the Apoenzyme - Unique features of Cobalt to suit Vitamin B12.

Copper Enzymes: Types of Copper in Biological Systems - Structural and Mechanistic Aspects of Superoxide Dismutase, Laccase and Galactose oxidase.
Molybdenum Enzymes: Biological Roles and Mechanistic Aspects of Nitrogenase, Xanthine oxidase and Sulfite oxidase.

SUGGESTED BOOKS

1. *Bioinorganic Chemistry*, Bertini, Gray, Lippard and Valentine, University Science Books, California USA 1994.
2. *Principles of Bioinorganic Chemistry,* S.J. Lippard and M.Berg University Science Books, Calfornia 1994.
3. *Biological Chemistry of Elements,* J.J.R. Franstodasilva and R.J.P. Williams Oxford University Press 1991.
4. *Metal Ions in Biological Systems* (Series), Ed. H. Sigel Marcel Dekkar, New York
5. *Inorganic Biochemistry,* J.A. Cowan, VCH publishers 1993.
6. *Advances in Inorganic Biochemistry,* edited by G.L.Eichorn & Marzilli
7. *Bioinorganic Chemistry,* Vol-I edited by G.L.Eichorn.

PAPER II

CH (IC) 402T: Medicinal Inorganic Chemistry

IC-29: Metal complexes as Drugs and Anticancer agents
IC-30: Metal complexes in Clinical Chemistry
IC-31: Chemical and Photochemical probing of DNA complexes
IC-32: DNA binding and molecular pharmacology and Interaction of Metallo Pharmaceuticals

IC-29: Metal complexes as Drugs and Anticancer agents

Introduction to Pt(II) chemistry – Thermodynamic and kinetic principles – *Cis* and *Trans* influences – Thermodynamic and kinetic aspects.

Platinum complexes in cancer therapy: Discovery applications and structure-effect Relationships. Cis platin(cis $Pt(NH_3)2Cl_2$) mode of action. Drug resistance and DNA repairmechanism.

Physical effects of metal complex: DNA binding, unwinding, shortening and bending of thedouble helix. Biological consequences of platinum –DNA binding. Organic intercalators asdonor – acceptor pairs; Transition metal complexes as donor acceptor pairs. Non classical platinum antitumour agents.

IC-30: Metal complexes in Clinical Chemistry

Theory and mode of action of therapeutic chelating agents , Single ligand Chelation Therapy –Aminopolycarboxylic acids, Desferrioxamine, pencillamine, triethylenetetramine, Mixed ligand chelation therapy - Metallothionens in detoxification. Role of metal ions in the action of antibiotics: Bleomycin, adriamyacin and tetracyclines. Gold-Containing drugs used in therapy of Rheumatoid arthritis - A therapeutic agent for Menkes disease: Copper-histidine - Anti viral chemotherapy and metal peptide interaction.

IC-31: Chemical and photochemical probing of DNA complexes

Chemical probing of DNA complexes: Introduction to foot printing. Chemical probing. Attack on DNA bases a) dimethylsulfate b) diethyl pyrocarbonate c) osmium tetraoxide d) aldehydes e) ethyl nitrosourea (ENA) and other chemical probes like tris phenanthroline metal complexes.

Photochemical probes: Psoralens, acridines, UV radiation Enzymatic probes

Immobilization of enzymes: Methods and Applications. Platinum Metal Complexes as drugs and anticancer agents: Importance of binding and photoreactive metal complexes, ligand dissociation and photoactive metal complexes, ligand dissociation and photosubstitution, photophysics and photochemistry of Ru(II) polypyridyl complexes. Photophysics and photochemistry of Ru(ii) polypiridyl complexes. Photophysics in the absence of DNA and in the presence of DNA.

IC-32: DNA binding and molecular pharmacology and Interaction of Metallo Pharmaceuticals

Introduction , concept of intercalating a) classical model b) developments of intercalation model c) quantitative analysis of intercalation.

Factors which relate intercalation and medicinal activity a) Binding constant b) kinetics c)structural effects and activities d) intercalation and drug action
Specific drugs which bind to DNA by intercalation : a) antipyranosomal drugs b) antimalarial drugs c) antitumor drugs. Nonspecific interaction in dye binding to DNA and influence of alcohols and amides. Ruthenium: Ru(III), amine complexes: Antitumor activity , structure activity relationship DNA binding and cleavage - DMSO complexes of Ru(II): DNA interactions of polyaromatic amines - Ru(IV) complexes oxidative DNA cleavage. Rhodium: Rhodium(II) acetate dimer. Anticancer activity metallocenes, Chemical correlation with antitumor activity, DNA binding and mechanistics possibility. Introduction, Structural and chemical properties of streptonigrin and its metal complexes - Evidence for formation of ternary complexes involving DNA and its components. Antitumor activity and mechanism - Metal induced free radical production by organic drugs in relation to their side effects.

SUGGESTED BOOKS

1. *Bioinorganic Chemistry. Inorganic elements in the Chemistry of life*, Wolfgang Kaim & Brigette Schwederdki.
2. *Handbook of Metal-Ligand interactions in Biological fluid Bioinorganic medicine*, Vol – 2 : Edt. Guy Berthon.
3. Bioinorganic Chemistry, Rosette M. Roat *Malone.*
4. *Photoreactions of Metal complexes with DNA,* A. Krisch – De Mesmacker et al.

PAPER III

CH(IC) 403T: Supra Molecular Chemistry and Bio Physical Studies

IC-33: Supramolecular Chemistry

IC-34: Structural aspects of DNA and RNA

IC-35: Spectroscopic analysis of drug/metal complexes binding to Nucleic acid:

IC-36: CD ,ORD, Fluorescence and Enzyme kinetics

IC-33: Supramolecular Chemistry

Basic Concepts of Host-Guest Complexation(Ionophore Chemistry)

General Principles of Molecular Recognition, Complex Formation and Host Design- Thermodynamics of Multi-Site Host-Guest Complexation: Macrocycles, Clefts and Open-chain Host Structures- Ionophores for Cations: Chelate, Macrocyclic and Cryptate Effects- Complexation Selectivity: the Hole-Size Concept and its Limitations- Enthalpy and Entropy Contributions and compensations- Heat Capacity Changes and Pre-organization- Ionophores for Anions: Macrocycles with secondary binding sites- Lariat Ethers, Ditopic Receptors, Cocomplexation and Second-sphere Coordination- Conformational Coupling Between binding sites: Cooperativily, Allosteric Effects and Induced Fit.

IC-34: Structural aspects of DNA and RNA

The covalent structure of polynucleotides, secondary structure of DNA : The double helix anti and syn conformations of nucleotides . B, A, & Z forms of DNA. Tertiary structure of DNA ; supercoiling, circuar and supercoiled DNA. The three kinds of RNA and their structures. Determination of primary structure of nucleic acids. (DNA & RNA). Recombinant DNA, Denaturation of DNA, helix coil transition, B-A transition, B-Z transition, study of thermal melting by UV absorption and infrared spectroscopy studies. Factors affecting the Tm. Metal DNA interactions: Influence of metal ions on stability of nucleic acids. Metal ions in genetic regulations.

IC-35: Spectroscopic analysis of drug/metal complexes binding to Nucleic acid

Absorption and Fluorescence spectra of drug – nucleic acid complexes, Salt back titrations interpretation of the data, cooperativity anticooperativity, the excluded site model, the binding analysis, equilibrium dialysis. Partition analysis, viscosity studies, competitive equilibrium dialysis to assess B & Z DNA binding . Obtaining equilibrium binding isotherms. Competition dialysis to assess base and sequence specificity. Dependence of Kobs on salt concentration, cation effects on Ligand nucleic acid equilibria, Competitive effects of monovalent and divalent cations for binding. Record's polyelectrolyte theory and its importance.

IC-36 : CD ,ORD, Fluorescence and Enzyme kinetics

Principles and instrumentation of CD and ORD spectroscopy. Cotton effect Use of CD in the conformational studies of metal complexes, DNA and DNA-metal complexes. Theory and principles of fluorescence spectroscopy. Characteristic of fluorescence emission, Fluorescence life time, quantum yield, Static and dynamic/collisional quenching and comparison.

Fluorescence polarization and polarization spectra of a fluorophore. Application of Fluorescence quenching in general and ligand/drug/metal complex DNA binding studies. Enzyme kinetics, Michaelis-Menton equation and its treatment, study state kinetic analysis, significance of Km and Kcat, Kcat/Km, effect of pH, temperature, substrate concentration. Types of enzyme inhibition,

SUGGESTED BOOKS

1. Biochemistry - Geoffrey L. Zubay.
2. Notes in Biochemistry – B.D. Hames, N.M. Hoopen & T.D. Houghfon.
3. Biochemistry - Mary K. Campbell.
4. Principles of fluorescence spectroscopes – Lakowicz.
5. Fluorescence Quenching theory and applications – Maurice R. Eftink.
6. Circular Dichroism Spectroscopes of DNA Methods in Enzymology Vol 211.
7. Tris (Phenanthroline) Metal complexes : probes for DNA Helicity
   Journal of Biomolecular structure and Dynamics Adenine Press 1983.
   G.L. Eichorn.8
8. Tris (Phenanthroline) Ru(II) Enantiomers interactions with DNA : Mode and
   specificity of binding J.B. Chaires. Biochemistry 1993 (32) 2573
9 . Spectroscopic Analysis of Drug. Nucleic acid interactions
   Geoffrey Dougherty & William J. Pigra.
10. Biophysical chemistry of Nucleic acids
   Victor A Bloomfield & D.M. Crothers.
11. Thermodynamics of Ligand – Nucleic acid Interactions
   T.M. Lohman, Methods in Enzymology Vol 212.
12 . Thermodynamic analysis of ion effects
   M.T. Record Biopolymers (1978).

PAPER IV (CB PAPER)

CH(IC) 404(CB_1)T: Separation Methods, Data Handling, Green Chemistry and Nanotechnology

IC (CB_1)-1: Separation Methods
IC (CB_1)-2: Data Handling
IC (CB_1)-3: Green Chemistry
IC (CB_1)-4: Nanotechnology

IC(CB_1)-1 : Separation Methods

Solvent extraction;The distribution coefficient ,distribution ratio, relation between Kd and D, The percent extracted. Solvent extraction of Metals- metal chelates ,Extraction process, analytical separations ,solid phase extraction.

Column Chromatography:Retention Parameters, Seperation efficiency, esolution,Asymmetric factor, Column efficiency,Column performance, HETP,Effective plate number , Van Deemeter Equation,

Gel Exclusion Chromatography: Principle, Stationary Phases, Instrumentation, Retention Behaviour, Applications.

Super Critical Fluid Chromatography: Principle, Super Critical Fluids, Instrumentation, Stationary Phases and Mobile Phases, Detectors, Comparison of SFC with HPLC and GC Applications.

IC(CB_1)-2 : Data Handling

Accuracy, Precision, Types of errors – determinate and indeterminate errors, minimization of determinate errors, statistical validation- statistical treatment of finite data (mean, median, average deviation, standard deviation, coefficient of variation and variance), significant figures – computation rules, comparision of results – student's t-test, F-test, statistical Q test for rejection of a result, confidence limit, regression analysis – method of least squares, correlation coefficient, detection limits. Calculations.

IC(CB_1)-3 : Green Chemistry

Principles and concepts of green chemistry

Introduction, sustainable development and green chemistry, atom economy, atom economic reactions, rearrangement reactions, addition reactions, atom uneconomic reactions- substitution reactions, elimination reactions, wittig reactions. Reducing toxicity, measuring toxicity.

Organic solvents: Environmentally benign solutions: Organic solvents and volatile organic compounds, solvent free systems, super critical fluids- supercritical carbon dioxide and supercritical water. Water as a reagent solvent, water based coatings.

Industrial case studies: A brighter shade of green – greening of acetic acid, Vitamin C synthesis –enzyme routes. Polythene manufacture-metallocene catalysis.

IC-(CB_1)-4 :Nanotechnology

Metal Nanoclusters

Magic numbers, theoretical modeling of nanoparticles, geometric structure, electronic structure, reactivity, fluctuations, magnetic clusters, bulk to nanotransition.

Methods of synthesis: RF plasma, chemical methods, thermolysis, pulsed laser methods.

Carbon nanostructures- Introduction, carbon molecules, new carbon structures,

Carbon clusters- small carbon clusters, discovery of C60, structure of C60 and its crystal, alkali doped C60, superconductivity in C60.
Carbon nanotubes: Fabrication, structure, electrical properties, vibrational properties, mechanical properties.
Applications of carbon tubes: Field emission and shielding, computers, fuel cells, chemical sensors, catalysis, mechanical reinforcement.
Biological Nanostructures: Examples of proteins, micelles and vesicles and multilayer films.

SUGGESTED BOOKS

1. Separation Methods - M. N. Sastri, 1st ed., Himalaya Publishers, 1991.
2. Principles of Instrumental Analysis – Skoog, Holler, Nieman, 5th ed., Harcourt College Publishers, 1998.
3. Analytical Chemistry - Gary D.Christian, 6th ed, John Wiley and sons. Inc., New York, sixth edition, 1994.
4. Green Chemistry- An Introductory text by Mike Lancaster- RSC.
5. Green Chemistry: Theory and Practice by John C. Warner Paul T. Anastas.
6. Introduction to nanotechnology by Charles P. Poole Jr, Frank J. Owens- Wiley Student Edition 2006.
7. Hand Book of Nanophase Materials by A.N. Gold Stein, ed, Marcel Decker, New York, 1997, Chapter 1.
8. Clusters of Transition Atoms" by Morse, Chem. Rev 86, 1049 (1986).
9. Hand Book of Nanostructured materials by P.M. Ajayan, H.S Nalwa, ed, Academic Press, San Diego, 2000, Vol. 5, chapter 6.

Paper –IV(CB_1 PAPER)

CH(IC) 404 (CB_2)T : Applied Analysis

IC (CB_2)-1: Data Handling
IC (CB_2)-2: Analysis of Air and Water Pollutants
IC (CB_2)-3: Clinical and Pharmaceutical analysis
IC (CB_2)-4: Food and Agricultural analysis

IC(CB_2) – 1 : Data Handling

Accuracy, Precision, Types of errors – determinate and indeterminate errors, minimization of determinate errors, statistical validation- statistical treatment of finite data (mean, median, average deviation, standard deviation, coefficient of variation and variance), significant figures – computation rules, comparision of results – student's t-test, F-test, statistical Q test for rejection of a result, confidence limit, regression analysis – method of least squares, correlation coefficient, detection limits. Calculations.

IC(CB_2) – 2 : Analysis of Air and Water Pollutants

Air quality standards, sampling, analysis of air pollutants-SO_2 (UV_Vis, IR), H_2S (Spectrophotometry and Non-dispersive IR Spectrophotometry), NO-NOx (Chemiluminescence technique, Colorimetric technique- Saltzman method), CO & CO_2 (IR, AAS & GC), Hydrocarbons (GC, GC-MS), Aromatic hydrocarbons in automobile exhaust, petrol, air, O_3 (Chemiluminiscence & Spectrophotometry), particulate matter analysis. Objectives of analysis, sampling, preservation and pre-concentration methods, physical analysis - colour, odour, temperature, pH, EC, redox potential, total desolved solids (turbidimetry), Chemical analysis of anions – CN-, Cl-, F-, NO_2-, NO_3- (spectrophotometry), SO_4, PO_4. Determination of BOD,COD, TOC & DO
Analysis of Toxic Metals: Hg, As, Pb, Cd, Be, Al, Cr (Atomic Absorption Spectroscopy and Spectrophotometry)

IC (CB_2)-3 : Clinical and Pharmaceutical Analysis

Clinical Analysis: Determination of (1) Serum Calcium (2) Serum/Plasma Bicarbonate (Titrimetry). Determination of Serum Chloride (Coulometry) - Determination of
(1) Cholesterol (2) Total Protein (3) Blood Urea in Serum (4) Amylase (5) Aspartate Amino Transferase (AST) and Alanine Amino Transferase (ALT) (by Spectrophotometry). Determination of (1) Thyroxin and (2) Thyroid-Stimulating Hormone (TSH) (by RIA Method)
Pharmaceutical analysis: Determination of Diclofenac (non-aqueous titration), Calcium in Vitamin D and Calcium formulations (Complexometry), Sulphanilamide (potentiometry), Pethidine hydrochloride (UV-Vis), Frusemide (UV-Vis), Aspirin,
paracetamol and codein in APC tablets (NMR), Phenobarbitone in tablets (IR), pivolic acid in dipivefrin eye drops (GC), Assay of hydrocortisone cream. (HPLC).
Impurity profiling of Propranolol (GC-MS), famotidine (LC_MS).

IC (CB_2) -4: Food and Agricultural Analysis

Food Analysis: Analysis of Chemical Additives in foods : Division of colour additives, Chromatographic identification of colours, and quantitative estimation of added dyes in foods (Titanium Trichloride Method) - chemical preservatives and synthetic sweetening agents

(Organic-ether extractable and Non-ether extractable) - Analysis of SO_2 & Sodium Benzoate (Chemical Methods), Sorbic Acid (Chromatography) - Types of Antioxidants used in Foods, Analysis of Butylated Hydroxy Toluene (BHT) (Spectrophotometry).

Agricultural Analysis: Analysis of soils for available Major Nutrients - Estimation of available Nitrogen (Kjeldahl Method), Phosphorus (Olsen's Method and Bray and Kurtz Method), and Exchangeable Calcium & Magnesium (by EDTA). Soil analysis for Micronutrients - Estimation of Available Zinc, Copper, Manganese and Iron (AAS) - Analysis of Pesticide Residues - Determination of Methyl Parathion Residues in food grains & vegetables (Solvent Extraction and Titrimetry) - Determination of Organochlorine pesticides by Gas Chromatography (Cypermethrin) - Determination of Malathion and DDT Residues in food grains (Spectrophotometry).

SUGGESTED BOOKS

1. Analytical Chemistry, Gary Christian, VI Ed, John Wiley & Sons Inc, New York.
2. Fundamentals of Analytcal Chemistry, Skoog & West.
3. Pharmaceutical Drug Analysis, Ashtoshka.
4. Vogel's Text Book of Quantitative Chemical Analysis, 6th Ed, Pearson Education Ltd.
5. Environmental Pollution Analysis, S M Khopkar, Wiley Eastern Ltd 1995.
6. Environmental Analytical Chemistry, F W Fifield, P J Haines, Blackie Academi Professional.
7. Environmental Chemistry, B K Sharma, Goel Publishing House, Meerut.
8. Handbook of Analysis and quality control for fruit and vegetable products, S Ranganna, Tata Mc Graw Hill Publishers Ltd, 1986.
9. Introduction to chemical analysis of foods, S Suzanna & Nielsen, CBS Publishers & Distributors.
10. Practical pharmaceutical Chemistry, a H Beckett and J B Stenlake, III Ed, Vol I and Vol II, CBS Publishers & Distributors,1997.
11. Pharmaceutical Analysis, David G Watson,Churchill Livingstone Harcourt Brace and Company Ltd, 1999.
12. Handbook of analysis of drugs, Nagavi.
13. Medical Laboratory Technology – Mukherjee , Tata Mc Graw Ltd 1988.
14. Medical Laboratory Technology – Ramnik Sood , Jaypee Brothers Ltd 1999.
15. Text Book of Clinical Chemistry V Edn Carl.A. Burtis Edward R. Ashwood Saunders Harcourt India 2001.

LABORATORY COURSES
PaperV: CH (IC) 451P: Spectroscopic techniques

(IC) 451P: Spectroscopic techniques
I Spectrophotometry
1. Estimation of manganese.
2. Estimation of chromium.
3. Simultaneous determination of Manganese and Chromium in a mixture.
4. Spectrophotometric Titrations of
   (i) Cu(II) with EDTA (ii) Bi(III) with EDTA (iii) Fe(II) with o-Phen
5. Determination of composition of Complex by Job's Method and Mole ratio Method in the following:
   (i) Cu(II)-EDTA (ii) Fe(II)-Bipyridyl (iii) Fe(II) with o-Phen

II Colorimetry
1. Determination of blood sugar
2. Determination of blood cholesterol
3. Determination of creatinine
4. Determination of Paracetamol

III Fluorimetry
1. Determination of Riboflavin
2. Determination of Quinine Sulphate.

IV Flame photometry
1. Determination of Na
2. Determination of K
3. Determination of Ca
4. Determination of Li

V Atomic Absorption Spectroscopy
1. Determination of i) Fe, ii) Mg, iii) Cu, iv) Pb.

References:

1. Text Book of Quantitative Inorganic Analysis Jaffery etal 4th edn. EdnElbs Publication
2. A Text Book of Quantitative Inorganic Analysis by A.I. Vogel 3rd EdnElbs Publication 1969.
3. Quantitative Analysis by Day and Underwood Prentice Hall (India) VI Edn.
4. Analytical Chemistry Thoery and Practice by R.M. Verma 3rd Edn.CBS Publishers & Distrbutors1994.
5. Practical Pharmaceutical Chemistry, A.H. Beckett and J.B. Stenlake 4thedn. CBS publishers, 2001
6. Medical Laboratory Technology – Mukherjee,Mc Graw Hills,1988

PaperVI: CH (IC) 452P: Structural Assignment of Metal Complexes from Physico-Chemical Data & Conventional Methods of Analysis I
Structural Assignment of Metal Complexes from Physico-Chemical Data
A complete characterization of the metal complex in terms of its composition, structure and other identification based on the following physico-chemical data given for each of the metal complexes will be made.
1. Elemental Analysis and other Physical Characteristics such as Conductivity, Dipole Moment, etc. (wherever available and applicable)
2. Infrared and Raman Spectra (Chart/Data)
3. NMR Spectra (Charts/Data based on *one* or *more* active nuclei)

4. Mossbauer Spectrum (Chart/Data, wherever applicable)
5. ESR Spectrum (Chart/Data, wherever applicable)
6. Electronic and CD/ORD Spectra (Charts/Data, wherever applicable)
7. Magnetic Susceptibility Data (at various temperatures if available)
8. CV and other Electrochemical Data
9. TGA/DTA Profiles
10. Any other Thermodynamic and Kinetic parameters that aid the structural assignment

II Conventional Methods of Analysis

i). Titrimetry:

1. Determination of Ca^{2+}, Mg^{2+}, CO_3^{2-}, HCO_3^- in soil sample
2. Determination of Iron & Calcium in Cement
3. Determination of saponification value of an oil sample
4. Determination of Iodine value of an oil sample
5. Determination of Calcium in calcium tablets

ii) Water analysis:

1. Determination of Dissolved Oxygen
2. Determination of COD
3. Determination of residual Chlorine in water by Iodometry
4. Determination of Fluoride by Zirconium Alizarin Method

SUGGESTED BOOKS

1. Chemistry Experiments for Instrumental Methods, Donald T Sawyer William R.Hememan etal John Wiley & Sons 1984.
2. Analytical Chemistry by Gary D.Christian 6th Edition John Wiley&Sons Inc New York 1994.
3. A Text Book of Quantitative Inorganic Analysis by A.I. Vogel 3rEdition Elbs Publication 1969.
4. Vogel's Text Book Of Quantitative Inorganic Analysis Jeffery etal 4th edition Elbs Publications 1988.
5. Vogel's Text Book of Quantitative Chemical Analysis, 6th edition. Pearson Education Ltd 2002.
6. Analytical Chemistry Thoery and Practice by R.M. Verma 3rd Edn.CBS Publishers & Distrbutors1994.
7. Comprehensive Experimental Chemistry by V.K. Ahluwalia etal New Age Publications 1997.
8.Laboratory hand Book of Instrumental Drug Analysis.by B.G. Nagavi 2nd edn. 1996

ORGANIC CHEMISTRY SPECIALISATION

SYLLABUS (2012 – 13) ONWARDS

III & IV SEMESTERS

M.Sc. CHEMISTRY(ORGANIC CHEMISTRY)

FOR STUDENTS ADMITTED IN THE YEAR (2011 – 12)

REVISED AS PER NEW (CB) SYLLABUS

M.Sc. CHEMISTRY(ORGANIC CHEMISTRY)
Syllabus for III and IV Semesters
(For the batch admitted during the academic year 2011-2012 under the CBCS pattern)

[Under Restructured CBCS Scheme]

(Approved in the P.G. BOS meeting held on 15-9-2012)

Semester - III

	Instruction Hrs/week	Internal assessment marks	Semester exam* marks	Total marks	Credits
CH(OC) 301T	4	20	80	100	4
CH(OC) 302T	4	20	80	100	4
CH(OC) 303T	4	20	80	100	4
CH(OC) 304T	4	20	80	100	4
SEMINAR	2	--	--	25	1
CH(OC) 351P	9	--	100	100	4
CH(OC) 352P	9	--	100	100	4
Total				**625**	**25**

*Theory: 3 hours; Practical's: 6 hours

Semester - IV

	Instruction Hrs/week	Internal assessment marks	Semester exam* marks	Total marks	Credits
CH(OC) 401T	4	20	80	100	4
CH(OC) 402T	4	20	80	100	4
CH(OC) 403T	4	20	80	100	4
CH(OC)404T (CB)	4	20	80	100	4
SEMINAR	2	--	--	25	1
CH(OC) 451P	9	--	100	100	4
CH(OC) 452P	9	--	100	100	4
Total				**625**	**25**

(**Choice based paper (CB) =** Paper offered by the same Department or other Department in the Science faculty)

*Theory: 3 hours; Practical's: 6 hours

Grand total (all 4 semesters) 2500 marks and 100 credits

PAPER TITLES

M.Sc. ORGANIC CHEMISTRY SPECIALISATION
III SEMESTER SYLLABUS
(For the batch admitted during the academic year 2011-2012 under the CBCS pattern)
[Under Restructured CBCS Scheme]

Paper 1– CH (OC) 301T: Conformational Analysis, Asymmetric Synthesis and Biomolecules

OC09: Conformational Analysis (cyclic systems)
OC10: Principles of Asymmetric synthesis
OC11: Methodologies in asymmetric synthesis
OC12: Biomolecules

Paper 2– CH (OC) 302T: Modern Organic Synthesis

OC13- Synthetic Reagents I
OC 14- Synthetic Reagents II
OC 15- New Synthetic reactions
OC 16- New techniques and concepts in organic synthesis

Paper 3: CH (OC) 303T: Organic Spectroscopy and Pericyclic reactions.

OC-17: ^{13}C NMR spectroscopy
OC-18: 2D NMR techniques and ORD
OC-19: Pericyclic reactions I
OC-20: Pericyclic reactions II

Paper-4 CH (OC) 304T: Photochemistry, synthetic strategies and Green Chemistry

OC-21 Photochemistry
OC-22 Synthetic strategies - I
OC-23 Synthetic strategies - II
OC-24 Green Chemistry

LABORATORY COURSES

PAPER-V CH (O) 351P: Separation and identification of organic compounds

PAPER VICH (O)352P: Synthesis of organic molecules & isolation of natural products

PAPER TITLES

M.Sc. ORGANIC CHEMISTRY SPECIALISATION

IV SEMESTER SYLLABUS

(For the batch admitted during the academic year 2011-2012 under the CBCS pattern)

[Under Restructured CBCS Scheme]

Paper-1 CH (OC) 401T: Drug Design and Drug Discovery

OC-25: Principles of Drug design and drug discovery
OC-26: Lead modification and SAR Studies
OC 27: QSAR studies
OC 28: Combinatorial Synthesis

Paper CH (OC) 402T: Drug synthesis and mechanism of action

OC-29: Drugs acting on metabolic process, cell wall and specific enzymes
OC-30: Drugs acting on genetic material and immune system
OC-31: Drugs acting on receptors and ion channels
OC-32: Chiral drugs

Paper-3 CH (OC) 403T: Advanced Heterocyclic Chemistry

OC-33: Non aromatic heterocyclics
OC-34: Five and six membered heterocyclics with two hetero atoms
OC-35: Heterocyclics with more than two hetero atoms
OC-36: Larger ring and other heterocycles

Paper-4 – CH (OC) 404(CB_1)T: Advanced Natural Products

OC(CB_1)-1: Biosynthesis of natural products
OC(CB_1)-2-: Structure determination and stereochemistry of natural products by chemical methods.
OC(CB_1)--3: Structure determination and stereochemistry of natural products by spectral methods.
OC(CB_1)--4: Total stereo selective synthesis of natural products.

Paper-4 CH (OC) 404T (CB_2): Bioorganic Chemistry

OC (CB_2) -1: Enzymes and their action
OC (CB_2) -2: Enzyme models and Enzymatic transformations
OC (CB_2) -3: Recombinant DNA and Fermentation technology
OC (CB_2) -4: Coenzymes

Paper-4 CH (OC) T404 (CB_3): Physical- Organic Chemistry

OC (CB_3) -1: MO and VB theory of reactivity
OC (CB_3) -2: Kinetic, isotopic, structural, solvent, steric and conformational effects
OC (CB_3) -3: Nucleophilic, electrophilic and free radical reactivity
OC (CB_3) -4: Supramolecular chemistry

Laboratory courses

PAPER-V CH(OC) 451P: Spectroscopic identification of organic compounds and Chromatography.

PAPER-VI CH(OC) 452P: Synthesis and analysis of drugs

M.Sc. ORGANIC CHEMISTRY SPECIALISATION
III SEMESTER SYLLABUS
(For the batch admitted during the academic year 2011-2012 under the CBCS pattern)
[Under Restructured CBCS Scheme]

Paper 1– CH (OC) 301T: Conformational Analysis, Asymmetric Synthesis and Biomolecules

OC09: Conformational Analysis (cyclic systems)
OC10: Principles of Asymmetric synthesis
OC11: Methodologies in asymmetric synthesis
OC12: Biomolecules

OC 09- Conformational analysis (Cyclic systems) 15 Hrs

Study of conformations of cyclohexane, mono, di and polysubstituted cyclohexanes, cyclohexene, cyclohexanone (2-alkyl and 3 -alkyl ketone effect), 2-halocyclohexanones, cyclopentane, cyclobutane, cycloheptane and cyclooctane, Stereo chemistry of bicyclo[3,3,0]octanes, hydrindanes, decalins and perhydroanthracenes. Conformational structures of piperidine, N-Methylpiperidine, tropane, tropine, pseudotropine, decahydroquinoline and quinolizidine. Conformaijonal effects on the stability and reactivity of diastereomers in cyclic molecules - steric and stereo electronic factors - examples Factors governing the reactivity of axial and equatorial substituents in cyclohexanes. Stereochemistry of addition to the carbonyl group of a rigid cyclohexanone ring.

OC l0- Principles of asymmetric synthesis 15 Hrs

Introduction and terminology: Topicity in molecules Homotopic, stereoheterotopic (enantiotopic and diastereotopic) groups and faces- symmetry, substitution and addition criteria.Prochirality nomenclature: Pro-R, Pro-S, Re and Si. Stereoselective reactions: Substrate stereoselectivity, product stereoselectivity, enantioselectivity and diastereoselectivity. Conditions forstereoselectivity: Symmetry and transition state criteria, kinetic and thermodynamic control. Methods for inducing enantio and diastereoselectivity. Analytical methods: % Enantiomeric excess, enantiomeric ratio, optical purity, % diastereomeric excess and diastereomeric ratio. Techniques for determination of enantiomeric excess, specific rotation, Chiral NMR; Chiralderivatizing agents, Chiral solvent, Chiral shift reagents and Chiral HPLC.

OC 11- Methodologies in asymmetric synthesis 15 Hrs

Strategies in Asymmetric Synthesis: l. Chiral substrate controlled, 2. Chiral auxiliary controlled, 3. Chiral reagent controlled and 4. Chiral catalyst controlled.

1. Chiral Substrate controlled asymmetric synthesis: Nucleophilic additions to chiral carbonyl compounds. 1, 2- asymmetric induction, Cram's rule and Felkin-Anh model.
2. Chiral auxiliary controlled asymmetric synthesis: α-Alkylation of chiral enolates, azaenolates, imines and hydrazones. 1, 4-Asymmetric induction and Prelog's rule. Use of chiral auxiliaries in Diels-Alder reaction.
3. Chiral reagent controlled asymmetric synthesis: Asymmetric reductions using BINAL-H. Asymmetric hydroboration using IPC_2 BH and $IPCBH_2$.
4. Chiral catalyst controlled asymmetric synthesis: Sharpless and Jacobsen asymmetric epoxidations. Sharpless asymmetric dihydroxylation. Asymmetric hydrogenations using chiral Wilkinson biphosphine and Noyori catalys. Enzyme mediated enantioselective synthesis
5. Asymmetric aldol reaction: Diastereoselective aldol reaction (chiral enolate & achiral aldehydes and achiral enolate & chiral aldehydes) its explanation by Zimmerman-Traxel model.

OC-12 Biomolecules **15 Hrs**

1. Enzymes: Definition. Classification based on mode of action. Mechanism of enzyme catalysis. Lock and Key model and Induced- Fit model. Enantiomer discrimination by Three-point Contact model. Factors affecting enzyme catalysis.Enzyme inhibition- reversible and irreversible inhibition. Enzymes in organic synthesis. Immobilised enzymes.
2. Nucleic acids: Primary, secondary and tertiary structure of DNA. Types of mRNA,tRNA and rRNA. Replication, transcription and translation. Genetic code. Protein biosynthesis. Chemical Synthesis of nucleosides and nucleotides.
3. Lipids: Lipid structure- acylglycerols, phosphoglycerides and sphingolipids. Biosynthesis of Lipids and chemical Synthesis of lipids.

Recommended Books:

1. Stereochemistry of organic compounds — Principles & Applications by D Nasipuri
2. Stereochemistry of Carbon compounds by Ernest L Eliel & Samuel H. wilen
3. Stereochemistry: Conformation & Mechanism by P S Kalsi
4. The third dimension in organic chemistry, by Alan Bassendale
5. Stereo selectivity in organic synthesis by R S Ward.
6. Asymmetric synthesis by Nogradi
7. Asymmetric organic reactions by J D Morrison and H S Moschcr
8. Principles in Asymmetric synthesis by Robert E. Gawley & JEFFREY AUBE
9. Stereo differentiating reactions by Izumi
10. Some modern methods of organic synthesis by W Carruthers
11. Guidebook to organic synthesis, by R K Meckie, D M Smith & R A Atken
12. Organic synthesis by Michael B Smith
13. Enzyme structure and mechanism by Fersht and Freeman
14. Bio-Organic chemistry by Hennan Dugas
15. Nucleic acids in Chemistry and Biology by G M Blackbum MI Gait
16. Lehninger Principles of Biochemistry by D L Nelson and M M Cox
17. Outlines of Biochemistry by Conn and Stumpf
18. Biotransformations in Organic Chemistry by K Faber.
19. Principles of biochemistry by Horton & others.
20. Bioorganic chemistry - A chemical approach to enzyme action by Herman Dugas and Christopher Penney.

Paper 2– CH (OC) 302T: Modern Organic Synthesis

OC13- Synthetic Reagents I

OC 14- Synthetic Reagents II

OC 15- New Synthetic reactions

OC 16- New techniques and concepts in organic synthesis

OC-13 Synthetic Reagents I — 15 Hrs

i) Protecting groups: a) Protection of alcohols by ether, silyl ether and ester formation b). Protection of 1,2-diols by acetal, ketal and carbonate formation c) Protection of amines by acetylation, benzoylation, benzyloxycarbonyl, t-butyloxycarbonyl, fmoc and triphenyl methyl groups. d) Protection of carbonyls by acetal, ketal and thiol acetal (Umpolung) groups. e) Protection of carboxylic acids by ester and ortho ester (OBO) formation.
ii) Oxidations: 1) Oxidation of active C-H functions: DDQ and SeO_2. 2) Alkenes to diols: Prevost and Woodward oxidation 3) Alcohol to carbonyls; Cr^{VI} oxidants (Jones reagent, PCC. PDC) IBX, DMP, CAN, TEMPO, TPAP, Swern oxidation 4). Oxidative cleavage of 1,2-diols: Periodic acid and Lead tetra acetate
iii) Reductions: a). Catalytic hydrogenation: Homogenous (Wilkinsons's catalytic hydrogenation) and heterogeneous catalytic reduction. b) Non-metallic reductions: Diimide reduction c) Dissolving metal reductions: Birch reduction. d) Nucleophilic metal hydrides: $LiAlH_4$, $NaBH_4$, and their modifications.e) Electrophilic metal hydrides: BH_3, AlH_3 and DIBAL. f) Hydrogenolysis g) use of tri-n-butyl tin hydride; Radical reductions.

OC-14: Synthetic Reagents II — 15 Hrs

i) Organometallic Reagents: a) Preparation and application of the following in organic synthesis: 1) Grignard, 2) Organo lithium and 3) Organo copper reagents b) Organo boranes in C-C bond formation c). Organo silicon reagents: reactions involving β-carbocations and α-carbanions, utility of trimethyl silyl halides, cyanides and triflates.
ii) Carbonyl methylenation: a) Phosphorous ylide mediated olefination: 1) Witting reaction, 2) Horner-Wordsworth-Emmons reaction b) Titanium- Carbene mediated olefination: 1) Tebbe reagent, 2) Petasis reagent c) Olefination by Nysted reagent

OC-15: New Synthetic reactions — 15 Hrs

1. Metal mediated C-C and C-X coupling reactions: Suzuki, Heck, Stille, Sonogishira cross coupling, Buchwald-Hartwig and Negishi-Kumada coupling reactions.
2. C=C Formation Reactions: Shapiro, Bamford-Stevens, McMurrey reactions, Julia-Lythgoe olefination and Peterson's stereoselective olefination.
3. Multicomponent Reactions: Ugi, Passerini, Biginelli, Hantzsch and Mannich reactions.

4. Ring Formation Reactions: Pausan-Khand reaction, Bergman cyclisation, Nazerov cyclisation.
5. Click Chemistry: Criteria for Click reaction, Sharpless azides cycloadditions.
6. Metathesis: Grubb's 1st and 2nd generation catalyst, Olefin cross coupling metathesis(OCM), ring closing metathesis(RCM), ring opening metathesis(ROM), applications.
7. Other important synthetic reactions: Baylis-Hilman reaction, Eschenmoser-Tanabe fragmentation, Mitsunobu reaction, Stork-enamine reaction and Michael reactions.

OC-16: New techniques and concepts in organic synthesis 15 Hrs

1. Techniques in peptide synthesis: Solid phase peptide synthesis, commonly used resins (Rink resin, Wang resin and Ellman resin, synthesis of cross linked Merrifield resin and drawbacks of solid phase synthesis.
2) Solid phase oligodeoxynucleotide synthesis: Triester pathway and phosphoramidite pathway
3) Oligosaccharide synthesis: Protection of hydroxyl groups, cylic oxocarbenium ion, glycosyl donors and glycosyl acceptors, Kahne glycosidation, convergent and linear oligosaccharide synthesis.
4) Phase Transfer catalysis: Onium and crwon ethers as PTC.
5) Tandem synthesis: Tandem reactions; conjugate addition-aldol reaction, polymerization-cyclisation, elctrocylic-Diels Alder reaction.
6) Baldwin Rules: Exo and Endo cyclisation, tetrahedral, trigonal and diagonal systems, favoured and disfavoured cyclisations.
7) Chiron approach in organic synthesis: Nature's chiral pool, carbohydrates, amino acids, hydroxy acids, terpenes as chiral precursors. Synthesis of shikimic acid from D-arabinose, furanonycin from D-glucose, S-(-)-ipsenol from S-leucine. 8) Determination of absolute configuration: Mosher's methods.

Recommended Books:

1. Some modern methods of organic synthesis by W. Carruthers
2. Guidebook to organic synthesis, by R K Meckie, D M Smith & R A Atken
3. Organic Synthesis by O House
4. Organic synthesis by Micheal B Smith
5. Reagents for organic synthesis, by Fieser & Fieser, Vol 1-11 (1984)
6. Organic synthesis by Robert E Ireland
7. Handbooks of reagents for organic synthesis by Reich and Rigby, Vol-I-IV
8. Total synthesis of natural products: the Chiron approach by S. Hanesian
9. Organic chemistry Jonathan Clayden, Nick Greeves and Stuart Warren

Paper 3: CH (OC) 303T: Organic Spectroscopy and Pericyclic reactions.

OC-17: ^{13}C NMR spectroscopy
OC-18: 2D NMR techniques and ORD
OC-19: Pericyclic reactions I
OC-20: Pericyclic reactions II

OC-17: ^{13}C NMR spectroscopy **15 Hrs**

CW and PFT techniques. Types of ^{13}C nmr spectra: undecoupled, proton- decoupled and off-resonance decoupled (ORD) spectra. ^{13}C chemical shifts, factors affecting the chemical shifts, chemical shifts of organic compounds. Calculation of chemical shifts of alkanes, alkenes and alkynes. Homonuclear (^{13}C, ^{13C} J) and heteronuclear (^{13}C,^{1}H J and ^{13}C- ^{2}H J) coupling. Applications of ^{13}C-NMR spectroscopy: Structure determination, stereochemistry, reaction mechanisms and dynamic processes in organic molecules. ^{13}C-NMR spectral editing techniques: principle and applications of APT, INEPT and DEPT methods.

OC-18 2D NMR techniques and ORD **15 Hrs**

1). 2D-NMR techniques: Principles of 2D NMR, Classification of 2D-experiments. Correlation spectroscopy (COSY) HOMO COSY (^{1}H-^{1}H COSY) , TOCSY (Total Correlation Spectroscopy), Hetero COSY (^{1}H,^{13}C COSY,HMQC), long range ^{1}H,^{13}C COSY (HMBC), Homonuclear and Heteronuclear 2D-J-resolved spectroscopy, NOESY and 2D-INADEQUATE experiments and their applications.

2) Optical Rotatory Dispersion (ORD) and CD Spectroscopy: Optical rotation, circular birefringence, circular dichroism and Cotton effect. Plain curves and anomalous curves. Empirical and semiempirical rules-The axial haloketone rule, the octant rule, Helicity rule, Exciton chirality method-Exciton coupling between identical chromophores. Benzene sector and chirality rule. Application of the rules to the study of absolute configuration and conformations of organic molecules.

OC-19 Pericyclic reactions I **15 Hrs**

Introduction - Characteristics and classification of pericyclic reactions— Electrocyclic, cycloaddition & cycloreversions and sigmatropic reactions—4ne and 4n+2e type examples.
Approaches for the interpretation of mechanism of pericyclic reactions-Aromatic Transition States (ATS)/Perturbation Molecular Orbitals (PMO) approach-Concept of Huckel –Mobius aromatic and antiaromatic transition states. Framing Woodward-Hofmann selection rules for all the pericyclic reactions by ATS approach. Solving problems based on ATS approach.

Aromaticity: Aromatic and anti aromatic compounds. Criteria for aromaticity. Huckel's 4n+2 electron rule for benzene and non benzenoid aromatic compounds. Eg. Cyclopropenium ion, cyclopentadienyl ion, cycloheptatrienium ion, azulene and annulenes.

OC-20 Pericyclic reactions II **15 Hrs**

Molecular orbitals-definition and their origin-Non-mathematical writing up of molecular orbitals and their symmetry properties for acyclic conjugated systems. Frontier Molecular Orbital (HOMO-LUMO) approach-concept-Framing Woodward-Hofmann selection rules for all the pericyclic reactions by Frontier Molecular Orbital (FMO) approach. Solving problems based on FMO approach. Conservation of orbital symmetry (Correlation Diagrams) approach-concept-Framing Woodward-Hofmann selection rules for electrocylic and cycloadditions & cycloreversions by Conservation of orbital symmetry approach.

Recommended Books :

1. Spectroscopic identification of organic compounds by RM Silverstein, G C Bassler and T B Morrill
2. Organic Spectroscopy by William Kemp
3. Spectroscopic methods in Organic chemistry by DH Williams and I Fleming
4. Modern NMR techniques for chemistry research by Andrew B Derome
5. NMR in chemistry - A multinuclear introduction by William Kemp
6. Spectroscopic identification of organic compounds by P S Kalsi
7. Introduction to organic spectroscopy by Pavia
8. Carbon-13 NMR for organic chemists by GC Levy and O L Nelson
9. Nuclear Magnetic Resonance Basic principles by Atta-ur-Rahman
10. Advanced organic chemistry. Part A Structure & Mechanism by Francis A. Corey and Richard J. Sundberg
11. Optical rotatory dispersion by C Djerassi
12. Optical rotatory dispersion and circular dichroism by P Crabbe
13. Mechanism and Structure in Organic chemistry by S Mukherjee
14. Advanced Organic Chemistry: Reactions, Mechanisms & Structure by Michael B Smith & Jerry March
15. Pericyclic Reactions by Mukherjee S M
16. Conservation of Orbital Symmetry by Woodward and Hoffmann
17. Organic Reactions and Orbital Symmetry, Gilchrist and Storr
18. Pericyclic Reactions — a problem solving approach, Lehr and Merchand
19. The Nature of Chemistry — Units 17-19 - Aromaticity — Open University, U K. Publications
20. The aromaticity III level, units 17-19 British open university volumes
21. Aromatic character and aromaticity by G.M.Badger
22. Non-benzenoid aromatic compounds by D.Ginsberg
23. Nonbenzenoid compounds by Lloyds

Paper-4 CH (OC) 304T: Photochemistry, synthetic strategies and Green Chemistry

OC-21 Photochemistry
OC-22 Synthetic strategies - I
OC-23 Synthetic strategies - II
OC-24 Green Chemistry

OC-21: Photochemistry **15Hrs**

Photochemistry of (π, π^*) transitions: Excited states of alkenes, cis-trans isomerisation, photostationary state, electrocyclisation and sigmatropic rearrangements, di-π methane rearrangement. Intermolecular reactions, photocycloadditions, photodimerisation of simple and conjugated olefins, addition of olefins to α, β-unsaturated carbonyl compounds. Excited states of aromatic compounds, Photoisimerisation of benzene

Photochemistry of (n-π^*) transitions: Excited states of carbonyl compounds, homolytic cleavage of α- bond, Norrish type I reactions in acyclic and cyclic ketones and strained cycloalkanediones.Intermolecular abstraction of hydrogen: photoreduction - influence of temperature, solvent, nature of hydrogen donor and structure of the substrate

Intramolecular abstraction of hydrogen:Norrish type II reactions in ketones, Esters and 1, 2-diketones, Addition to carbon-carbon multiple bonds, Paterno-Buchi reaction, Photochemistry of nitrites-Barton reaction.

OC-22: Synthetic Strategies I **15 Hrs**

Synthetic Strategies; Introduction, Terminology: target, synthon, synthetic equivalent, functional group interconversion (FGI), functional group addition, functional group elimination. Criteria for selection of target. Linear and convergent synthesis. Retrosynthetic analysis and synthesis involving chemoselectivity, regioselectivity, reversal of polarity and cyclizations. . Order of events in synthesis by retrosynthetic approach, explanation with examples S-salbutamol, Propoxycaine and Dinocap. Introduction to one group C-C and C-X disconnections. One group C-C disconnections, Alcohols and carbonyl compounds. One group C-X disconnections ,Carbonyl compounds, alcohols, ethers and sulphides.

OC-23: Synthetic Strategies II **15 Hrs**

Introduction to two group C-C and C-X disconnections , Two group C-X disconnections; 1,1-difunctionalised, 1,2-difunctionalised and 1,3-difunctionalised compounds. Two group C-C disconnections; Diels-Alder reaction, 1,3-difunctionalised compounds, 1,5- difunctionalised compounds, Michael addition and Robinson annulation. Control in carbonyl condensations, explanation with examples oxanamide and mevalonic acid. Strategic bond: definition, choosing disconnection/ guidelines for disconnection; disconnection of C-X bonds, disconnect to greatest simplification, using symmetry in disconnection, disconnection corresponding to known reliable reaction, high yielding steps and recognizable starting materials. Other approaches to retro

synthesis – biomimetic approach (Johnsons polyene cyclisation), and retro mass spectral fragmentation. Application of the strategies to the synthesis of (+) Disparlure, Retronecene, longifoline.

OC-24: Green Chemistry **15Hrs**

Introduction. Principles, atom economy and scope. Introduction to alternative approaches.

1. Solvent free reactions-principle, scope, utility of solvent free condition reactions.
Organic Synthesis in solid state (without using any solvent): Michael addition, Beckmann rearrangement, Synthesis of aziridines; solid supported organic synthesis: Synthesis of aziridines, pyridines, chromenes and flavones.

2. Aqueous Phase Reactions: Diels-Alder Reaction, Heck reaction, epoxidation, Dihydroxylation (Syn- & Anti-)

3. Microwave Technology: Microwave equipment, activation-benefits, limitations, microwave effects.

a) Microwave Solvent free reactions (Solid state Reactions) - Deacetylation, deprotection, saponification of esters, alkylation of reactive methylene compounds, synthesis of nitriles from aldehydes, reductions.

b) Microwave assisted reactions in water — Hoffmann elimination, hydrolysis, oxidation, saponification reactions.

c) Microwave assisted reactions in organic solvents — Esterification reactions, Fries rearrangement, Orthoester Claisen rearrangement, Diels- Alder reaction, decarboxylation.

d) Microwave assisted reactions under PTC conditions:

4. Ultrasound assisted reactions: introduction, substitution reactions, addition, oxidation, reduction reactions.

5. Organocatalysis: Aldol reactions, Acyl transfer reactions, nucleophilic N-heterocyclic carbenes in asymmetric organocatalysis, setter reaction and Baker's Yeast.

6. Ionic liquids: Introduction and applications in organic synthesis (illustrate with two examples).

Recommended Books

1. Green chemistry, Theory and Practical, Paul T.Anastas and John C.Warner.
2. New trends in green chemistry By V.K.Ahulwalia and M.Kidwai.
3. Organic Synthesis: Special techniques. V.K.Ahulwalia and Renu Aggarwal.
4. Enantioselective organocatalysis, Peter I Dallco, Willey-VCH.
5. Molecular Reactions and Photo chemistry by Depuy and Chapman
6. Photochemistry by C W J Wells
7. Organic Photochemistry by Turro
8. Molecular Photochemistry by Gilbert & Baggo
9. Organic Photochemistry by D Coyle
10. Organic Synthesis-The disconnection approach by S Warren
11. Organic Synthesis by C Willis and M Willis
12. Problems on organic synthesis by Stuart Warren

Semester III
Laboratory courses

Paper CH (O) 351P: Separation and identification of organic compounds

Separation of two component mixtures by chemical methods and their identification by chemical reactions — separation by using solvent ether, 5 % aqueous sodium bicarbonate, 5% sodium hydroxide and dil hydrochloric acid, checking the purity of the two components by TLC, identification of the compounds by a systematic study of the physical characteristics (mp/bp), extra elements (nitrogen, halogens and sulfur), solubility, functional groups, preparation of crystalline derivatives and identification by referring to literature. A minimum of 10 mixtures should be separated and analyzed by these procedures.

Separation of three component mixtures by chemical methods. A minimum of two mixtures should be separated and analyzed.

Paper CH (O) 352P: Synthesis of organic molecules & isolation of natural products

(A) Laboratory synthesis of the following compounds:

2-Phenyl indole (Fischer indole synthesis), 7-hydroxy-3-methyl flavone (Baker - Venkatraman reaction), 2,5-Dihydroxy acetophenone (Fries reaction), 4- Chlorotoluene from p-toluidine (Sandmeyer reaction), Benzilic acid from benzoin (Benzillic acid rearrangement), Benzpinacol (photochemical reaction), 7-hydroxy coumarin (Pechman synthesis), Photo-dimerization of maleic anhydride, benzophenone (Friedel-Crafts reaction), Benzanilide (Beckmann rearrangement), Vanillyl alcohol from vanillin ($NaBH_4$ reduction), 2- and 4-nitrophenols (nitration and separation by steam distillation), Acridone from Phthalic anhydride.

(B) Isolation of the following natural products:

Caffeine from tea leaves (solvent extraction), Piperine from pepper (Soxhlet extraction), Eucalyptus oil from leaves (steam distillation), Lycopene from tomatoes.

Recommended Books:

1. Practical organic chemistry by Mann & Saunders
2. Text book of practical organic chemistry by Vogel
3. The systematic identification of organic compounds by Ralph L. Shriner, Christine K. F. Hermann, Terence C. Morrill and David Y. Curtin

M.Sc. CHEMISTRY(ORGANIC CHEMISTRY)
IV SEMESTER SYLLABUS
(For the batch admitted during the academic year 2011-2012 under the CBCS pattern)
[Under Restructured CBCS Scheme]

Paper-1 CH (OC) 401T: Drug Design and Drug Discovery

OC-25: Principles of Drug design and drug discovery
OC-26: Lead modification and SAR Studies
OC 27: QSAR studies
OC 28: Combinatorial Synthesis

OC- 25: Principles of Drug design and drug discovery **15 Hrs**

Introduction to drug discovery. Folklore drugs, stages involved in drug discovery- disease, drug targets, bioassay. Discovery of a lead- screening of natural products and synthetic compound libraries. Existing drugs as leads (me too drugs). Pharmacokinetics (ADME), pharmacodynamics. Nature of drug – receptor interactions and their theories – Occupancy theory, Induced – fit theory, Macromolecular purturbation theory and Two-state model of receptor activation. Natural products as lead structures in drug discovery – Pharmacophore - structure pruning technique e.g. morphine. Discovery of lead structure from natural hormones and neurotransmitters. Principles of design of agonists (e.g.Salbutamol), antagonists e.g. cimitidine) and enzyme inhibitors (e.g. captopril). Drug discovery without lead – serendipity- Penicillin and Librium as examples. Principles of prodrug design. Introduction to drug patents and Clinical trials.

OC-26: Lead modification and SAR Studies **15 Hrs**

SAR: Lead modification strategies, Bioisosterism, variation of alkyl substituents,chain homologation and branching, variation of aromatic substituents,extension of structure, ring expansion and ring contraction, ring variation, variation and position of hetero atoms, ring fusion, simplification of the lead, rigidification of lead.Discovery of oxaminquine, salbutamol, cimitidine and captopril Structure-Activity Relationship studies in sulfa drugs,benzodiazepines, and taxol analogs.

OC-27: Quantitative Structure- Activity Relationship (QSAR) studies **15 Hrs**

Introduction, physicochemical properties - pKa, electronic effects and Hammett constants(σ), lipophilicity constant(π), steric effects and Taft's constant, linear and nonlinear relationship between biological activity and Hammett/ Lipophilicity Substituent constants. Lipenski rule of five. Hansch analysis, Craig's plot,Topliss scheme, Free Wilson approach, cluster significant analysis. Three case studies. Principles of molecular modeling in drug design.

OC-28: Combinatorial Synthesis **15Hrs**

Introduction. Combinatorial approach. Combinatorial libraries, technologies. Solid phase synthesis, types of resins. Linkers. Reactants for solid phased synthesis. Methods of Parallel synthesis: Haughton's tea bag procedure. Automated parallel synthesis. Methods in Mixed combinatorial synthesis: general principles. Furkas mix and split combinatorial synthesis, Structure determination of active compounds-Deconvolution, Methods in deconvolution-recursive deconvolution, tagging and use of decoded sheets. Examples of Combinatorial Chemistry. Planning and designing of combinatorial synthesis, Spider like scaffolds, drug molecules. Automation in Combinatorial chemistry. High throughput screening.

Recommended books

1. Burger's medicinal chemistry and drug discovery by Manfred E. Wolf.
2. Introduction to Medicinal chemistry by Patrick.
3. Introduction to drug design by R Silverman
4. Comprehensive medicinal chemistry. Vol 1-5 by Hanzsch.
5. Principles of medicinal chemistry. by William Foye
6. Biochemical approach to medicinal chemistry. by Thomas Nogrady.
7. Pharmaceutical Chemistry and Drug synthesis by Roth and Kleeman
8. Drug design by E.J.Arienes
9. Principles of Medicinal Chemistty Vol I & II by Kadam et al
10. Medicinal chemistry An introduction by Garreth Thomas
11.Organic and Pharmaceutical chemistry By Delgrado
12. Organic Pharmaceutical chemistry By Harikishan singh
13. Medicinal Chemistry By Ashtoshkar
14. Medicinal Chemistry By Chatwal
15. Organic Drug synthesis By Ledneicer Vol 1-6
1 6.Strategies for organic drug synthesis and design By Daniel Ledneicer.
1 7.Top Drugs: Top synthetic routes By John Saunders
I 8.Chirotechnoiogy By Roger A. Sheldon
19. Burger's Medicinal Chemistry and Drug Discovery: Principles and Practices. Vol. 1.
20. Medicinal Chemistry by G. Patricks.
21. Text book of Drug Design and Discovery, Edited by Povl Krogsgaard – Larsen Tommy Liljefors.
22. Structure Based Drug Design of Crizotinib (PF-02341066), a Potent and Selective Dual Inhibitor of Mesenchymal–Epithelial Transition Factor (c-MET) Kinase and Anaplastic Lymphoma Kinase (ALK) Martin P. Edwards, J. Med. Chem., 2011, 54 (18), pp 6342–6363. http://www.pfizer.com/news/featured_stories/featured_stories_martin_edwards.jsp

Paper CH (OC) 402T: Drug synthesis and mechanism of action

OC-29: Drugs acting on metabolic process, cell wall and specific enzymes
OC-30: Drugs acting on genetic material and immune system
OC-31: Drugs acting on receptors and ion channels
OC-32: Chiral drugs

OC-29: Drugs acting on metabolic process, cell wall and specific enzymes

Basic concepts of mechanism of drug action: Introduction to macromolecular targets, carbohydrates, proteins, lipids and nucleic acids as possible drug targets. Classification of drugs. Enzyme inhibition and its types.

a**)** Drugs acting on metabolic process:

Antifolates –Discovery and mechanism of action of sulphonamides, Synthesis of sulfomethoxazole, sulfodoxine, sulfaguanidine and dapsone.

Diaminopyrimidines -trimethoprim, bacterial resistance to sulfonamides and drug synergism

b**)**Drugs acting on cell wall: Structure of bacterial cell wall, β-Lactam antibiotics – mechanism of action of penicillins and cephalosporins. Synthesis of pencillin-G and cephalosporin-C, cefalexin and cycloserine. Resistance to pencillins, broad spectrum penicillins – cloxacillin, methicillin, ampicillin, amoxicillin and carbenicillin. β-Lactamase inhibitors - Structural formulae and mode of action of clavulanic acid and sulbactum

c)Drugs acting on specific enzymes: H^+/K^+ -ATPase inhibitors- synthesis of Omeprazole and Carbonic anhydrase inhibitors-synthesis of Acetazolamide.

OC-30: Drugs acting on genetic material and immune system

Drugs acting on genetic material: Introduction, classification and mechanism of action.

a) DNA-intercalating agents-Anticancer and antimalarial agents. Structural formulae of Daunomycin, Adriamycin and Amsacrine. Synthesis of Amscarine, Nitracrine, Quinacrine and Chloroquine.

b) DNA- Binding and nicking agents: Antiprotozoal drugs. Synthesis of Metronidazole, Dimetridazole and Tinidazole.

c) DNA-Alkylators: Synthesis of Cyclophosphamide and Bisulphan.

d) DNA-Polymerase inhibitors: Antiviral agents- Synthesis of Acyclovir and AZT.

e) DNA-Topoisomerase inhibitors: Anti bacterial agents. Synthesis of Ciprofloxacin and Norfloxacin. Structural formulae of loxacin and Lomefloxacin.

f) Inhibitors of transcribing enzymes: Anti-TB and antileprosy agents-structural formulae of Rifamycins and partial synthesis of Rifampicin.

g) Drugs interfering with translation process: Antibacterial drugs- Structural formulae of Erythromycin, 5-Oxytetracycline and Streptomycin. Synthesis of Chloromycetin

Drugs acting on immune system: Introduction to immune system. Immunosupressing agent-structural formula of Cyclosporin. Immunoenhancers-use of vaccines and strucrural formula of levamisol.

OC-31: Drugs acting on receptors and ion channels

Introduction to nervous system: structure of neuron, nerve transmission. Definition and examples of agonist, antagonist, neurotransmitters and receptors.

Drugs acting on receptors:

a)Adrenergic receptors - Introduction and classification. α-Adrenergic-receptor agonists and antagonists- Synthesis and biological activity of Nor-adrenaline, Methyl L dopa and Tetrazosin. β-Adrenergic-receptor - agonists and antagonists – Synthesis and pharmacological activity of Salbutamol, Tetrabutalin, Propranolol and Atenolol.

b)Cholinergic-receptors: Introduction and classification. Cholinergic-receptor agonists and antagonists- Structural formulae of Nicotine, Atropine and Tubocurarine. Synthesis of Acetyl choline and Succinyl choline

c)Dopamine receptors: Introduction and classification. Dopamine- receptor agonists and antagonists- Biosynthesis of Dopamine. Synthesis of L-Dopa and Chlorpromazine.

d)Serotonin receptors: Introduction and classification. Serotonin receptor agonists and antagonists-synthesis and pharmacological activity of Serotonin and Metoclopramide.

e)Histamine receptors: Introduction and classification. Histamine receptor agonists and antagonists-synthesis and biological action of Histamine, Chloropheneramine, and Ranitidine.

f) Hormones and their receptors: Introduction to estrogen receptors, Structural formulae of Tamoxifen

Drugs acting on ion channels: Introduction to ion channels, drugs acting on Ca^{2+}, Na^{+} and Cl^{-} channels and their mode of action. Structural formulae of Tetracaine and synthesis and of Nifedipine, Diltiazem, Tetracine and 4-Aminopyridine.

OC-32: Chiral drugs

Introduction to chiral drugs. Three-point contact model, Eutomer, Distomer and eudesmic ratio. Pfeiffer's rule. Role of chirality on biological activity: Distomers – a) with no side effects b)with undesirable side effects c) both isomers having independent therapeutic value d)combination products having therapeutic advantages e) metabolic chirality inversion.

Synthesis and pharmacological activity of S-Ibuprofen, S- Metaprolol, Ininavir sulfate, Levocetrazine, 2S-Verapamil, S,S-Ethambutol , (+)Lomefloxacin, Fluvastatin, Dextropropoxyphen, (+)Ephedrine, (+)Griseofulvin, Dexormaplatin, R-Indacrinone, Nateglinide, Oxybutynin hydrochloride, S,S- Captopril and S,S,S- Enalaprilate.

Recommended Books:

1. Burger's medicinal chemistry and drug discovery. By Manfred B. Wolf.
2. Introduction to Medicinal chemistry. By Graham Patrick.
3. Introduction to drug design. By R.B.Silverman
4. Comprehensive medicinal chemistry. Vol 1-5 by Hanzsch.
5. Principles of medicinal chemistry. By William O. Foye etal.
6. Biochemical approach to medicinal chemistry. By Thomas Nogrady.
7. Pharmaceutical Chemistry and Drug synthesis By Roth and Kleeman
8. Drug design By E.J. Arienes
9. Principles of Medicinal Chemistry. Vols.1 & 2 By Kadam etal
10. Medicinal chemistry An introduction By Gareth Thomas

11. Wilson and Gisvold,s text book of Organic, Medicinal and Pharmaceutical chemistry By J.N.Delgado and W.A.Remers.
12. Organic Pharmaceutical chemistry By Harikishan singh.
13. Medicinal Chemistry By Ashutoshkar
14. Medicinal Chemistry By G.Chatwal
15. Organic Drug synthesis By Ledneiser Vol 1-6
16. Strategies for organic drug synthesis and design By Daniel Ledneiser
17. Top Drugs: Top synthetic routes By John Saunders
18. Chirotecchnology By Roger A. Sheldon

Paper-3 CH (OC) 403T: Advanced Heterocyclic Chemistry

OC-33: Non aromatic heterocyclics
OC-34: Five and six membered heterocyclics with two hetero atoms
OC-35: Heterocyclics with more than two hetero atoms
OC-36: Larger ring and other heterocycles

OC-33: Nonaromatic heterocyclics **15 Hrs**

Different types of strains, interactions and conformational aspects of nonaromatic heterocycles. Synthesis, reactivity and importance of the following ring systems. Azirines, Aziridines, Oxiranes, Thiiranes, Diazirenes, Diaziridines, Oxaziridines, Azetidines, Oxetanes and Thietanes

OC-34: Five and six membered heterocyclics with two hetero atoms **15 Hrs**

Synthesis, reactivity, aromatic character and importance of the following heterocycles: Pyrazole, Imidazole, Oxazole, Thiazole, Isoxazole, Isothiazole, Pyridazine, Pyrimidine. Pyrazine, Oxazine, thiazine, benzimidazole, benzoxazole and benzthiazole.

OC-35: Heterocyclics with more than two hetero atoms **15 Hrs**

Synthesis, reactivity, aromatic character and importance of the following Heterocycles: 1,2,3-triazoies,1,2,4-triazoles, Tetrazoles, 1,2,4-oxadiazole, 1 ,3,4-oxadiazole, 1,2,5- oxadiazole, 1,2,3-thiadiazoles, 1,3,4- thiadiazoles, 1,2,5- thiadiazoles, 1,2,3-triazine, 1,2,4- triazine, 1,3,5- triazine, tetrazines. Synthesis and importance of purines and pteridines. Syntheis of Caffeine, theobromine and theophylline.

OC-36: Larger ring and other Heterocycles **15 Hrs**

Synthesis, structure, stability and reactivity of Azepines, Oxepines and Thiepines. Synthesis of Diazepines rearrangements of 1,2 - diazepines. Synthesis of Benzoazepines, Benzodiazepines, Benzooxepines, Benzothiepines, Azocines and Azonines. Synthesis of selenophenes, Tellerophenes, Phospholes and Boroles.

Recommended Books:

1. Heterocyclic Chemistry, T.Gilchrist
2. An introduction to the Chemistry of heterocyclic compounds, R.M.Acheson
3. Heterocyclic Chemistry, J.A.Joule & K.Mills
4. Principles of Modern Heterocyclie Chemistry, A.Paquette
5. Heterocyclic Chemistry, J,A.Joule & Smith
6. Handbook of Heterocyclic Chemistry, A.R.Katritzky

Paper-4 – CH (OC) 404T(CB_1): Advanced Natural Products

OC(CB_1)-1: Biosynthesis of natural products

OC(CB_1)-2-: Structure determination and stereochemistry of natural products by chemical methods.

OC(CB_1)--3: Structure determination and stereochemistry of natural products by spectral methods.

OC(CB_1)--4: Total stereo selective synthesis of natural products.

OC(CB_1)-1: Biosynthesis of natural products 15 Hrs

Biosynthesis of secondary metabolites: Introduction, Difference between Laboratory synthesis and biosynthesis. Methods for determination of biosynthetic mechanism. Isolation and identification of Biosynthetic precursors, Feeding experiments – use of radioisotopes Measurement of incorporation – absolute incorporation, specific incorporation. Identification of the position of labels in labeled natural products by chemical degradation and spectral methods. Major biosynthetic pathways: 1) Acetate-Malonate pathway: Biosynthesis of aromatic compounds, 2) Shikimic acid pathway ; Biosynthesis of essential amino acids – phenylalanine, tyrosine and tryptophan, carboxylic acid derivatives, flavonoids and morphine alkaloids. 3) Mevalonic acid pathway : Biosynthesis of terpenes – mono, sesqui, di, tri (β-amyrin) and carotenoids, steroids – cholesterol.

OC(CB_1)-2: Structure determination and stereochemistry of natural products by chemical methods 15 Hrs

Determination of structure and stereochemistry of morphine, reserpine, abietic acid, cholesterol and rotenone.

OC(CB_1)-3: Structure determination and stereochemistry of natural products by spectral methods 15 Hrs

Spectroscopic techniques IR, UV, ^{1}Hnmr, ^{13}Cnmr, COSY, HETEROCOSY, NOESY, 2D-INADEQUATE and MS in the structure elucidations of natural products, Examples, flavones, biflavones, flavanones, isoflavones, coumarins, quinolines, isoquinolines.

Study of the following solved problems: Mass, IR, ^{1}H, ^{13}C NMR, HOMOCOSY, HECTOR, DEPT, 2D-INADEQUATE and NOE of Geraniol, INEPT of **menthol**, APT of **apparicine**, Heteronuclear 2D-J resolved spectrum of **stricticine**, NOESY of **buxaquamarine**, HETEROCOSY of **strictanol**, 2D-INADEQUATE of **α-picoline** and **β-methyl tetrahydran furan**.

OC(CB_1)-4: Total stereoselective synthesis of natural products. 15 Hrs

Woodward's synthesis of reserpine and cholesterol, Corey's synthesis of prostaglandins (E2, F2α) and paeoriflorin, Sharpless synthesis of L-hexoses, Nicolaous synthesis of taxol,

Danishefsky synthesis of indolizomycin, Takasago synthesis of menthol, Hoffmann-LaRoche synthesis of Biotin.

Recommended books:

1. Textbook of organic chemistry, Vol II by I L Finar
2. Chemistry of natural products, Vol 12, by Atta-Ur-Rahman
3. An introduction to the chemistry of terpenoids and steroids, by William templeton
4. Systematic identification of flavonoid compounds by Mabry & Markham
5. Steroids by Fieser arid Fieser
6. Alkaloids by Manske
7. Alkaloids by Bentley
8. The chemistry of terpenes by A Pinder
9. The terpenes by Simenson
10. Terpenoids by Mayo
11. Alkaloids by Pelletier
12. Total synthesis of Natural Products by Apsimon Vol 1-5
13. Biosynthesis by Geismann
14. Principles of organic synthesis 3rd Ed.R O C Norman and J M Coxen
15. One and two dimensional nmr spectroscopy by Atta Ur Rahman
16. Classics in total synthesis K C Nicolaou and E J Sorenson
17. Spectrometric identification of organic compounds by Silverstein and Webster

Paper-4 CH (OC) 404 T(CB_2): Bioorganic Chemistry

OC (CB_2) -1: Enzymes and their action
OC (CB_2) -2: Enzyme models and Enzymatic transformations
OC (CB_2) -3: Recombinant DNA and Fermentation technology
OC (CB_2) -4: Coenzymes

OC (CB_2)-1: Enzymes and their action — 15 Hrs

Introduction to enzymes. Transition state theory. Acid-Base catalysis. Covalent catalysis— Binding modes of catalysis (i) Proximity effect (ii) Transition state stabilization (iii) Strain and Distortion. Examples of some typical enzyme mechanisms for (1) Triose phosphate isomerase, (ii) α-chymotrypsin and serine protease (iii) Lysozyme (iv) Carboxy peptidase-A (v) Ribonuclease.

OC (CB_2)-2: Enzyme Models and Enzymatic transformations — 15 Hrs

Introduction — Biomimetic chemical approach to biological systems-Enzyme models Advantage of enzyme models. Requirements necessary for the design of enzyme models. Host-Guest complexation chemistry. Examples of some host molecules-Crown ether cryptanes, cyclodextrins. Cyclodextrin based enzyme models-Valixarenes, ionophores, micelles and synzymes (synthetic enzymes) — chiral recognition and catalysis.Introduction to industrial enzymes. Enzymatic synthesis of α-amino acids and peptides. Transformations of lipases and esterases. Kinetic resolutions of catboxylic acids, esters and alcohols - Transesterification. Amine resolution-use of oxido-reductase. C-C bond formation using enzymes-asymmetric cyanohydrin formation and asymmetric aldol condensations.

OC (CB_2) -3: Recombinant DNA and Fermentation technology — 15 Hrs

Introduction to genetic engineering. Recombinant DNA technology-restriction endonuclease, cloning, linkers, adaptors. Application of recombinant DNA technology in production of pharmaceuticals, diagnosis of diseases, insect control, improved biological detergents, gene therapy-examples. Principles of finger printing technology- Site directed mutagenesis. Fermentation technology: Introduction to fermentation. Industrial fermentation. Advantages and limitations of fermentation. Production of drugs and drug intermediates from fermentation-examples. Chiral hydroxy acids, vitamins, amino acids, β-lactam antibiotics. Precursor fermentation and microbial oxidation and reductions.

OC (CB_2) -4: Coenzymes — 15 Hrs

Introduction. Co factors — cosubstrates — prosthetic groups. Classification — Vitamin derived coenzymes and metabolite coenzymes.Structure and biological functions of coenzyme A, thiamine pyrophosphate (TPP), pyridoxal phosphate (PLP), oxidized and reduced forms of I) nicotinamide adenosine dinucleotide / their phosphates (NAD), NADH, $NADP^+$ NADPH) ii) Flavin adenine nucleotide FAD, $FADH_2$ and iii) Flavin mononucleotide (FMN, $FMNH_2$) lipoic

acid, biotin, tetrahydrofolate and ubiquinone. Adenosine triphosphate (ATP) and adenosine diphosphate (ADP), S-adenosyl methionine (SAM) and uridine diphospho sugars (UDP-sugars) Mechanism of reactions catalyzed by the above coenzymes.

Recommended Books

1. Concepts in biotechnology by D. Balasubramananian & others
2. Principals of biochemistry by Horton & others.
3. Bioorganic chemistry - A chemical approach to enzyme action by Herman Dugas and Christopher Penney.
4. Chirotechnology by R.Sheldon

Paper-4 CH (OC) 404 T(CB_3): Physical- Organic Chemistry

OC (CB_3) -1: MO and VB theory of reactivity

OC (CB_3) -2: Kinetic, isotopic, structural, solvent, steric and conformational effects

OC (CB_3) -3: Nucleophilic, electrophilic and free radical reactivity

OC (CB_3) -4: Supramolecular chemistry

OC (CB_3) -1- Molecular Orbital (MO) and Valence Bond (VB) theory of reactivity

Introduction to Huckel molecular orbital (MO) method as a means to explain modern theoretical methods. Advanced techniques in PMO and FMO theory. Molecular mechanics, semiemperical methods and ab inito and density functional methods. Scope and limitations of several computational programmes. Quantitative MO theory-Huckel molecular orbital (HMO) method as applied to ethane energy levels .Orbital symmetry, orbital interaction diagrams. MO of simple organic systems such as ethane, allyl, butadiene, methane and methyl group. Conjugation and hyperconjugation. Aromaticity. Valence bond (VB) configuration mixing diagrams. Relationship between VB configuration mixing and resonance theory. Reaction profiles. Potential energy diagrams. Curve crossing model nature of activation barrier in chemical reactions. Principle of reactivity Mechanistic significance of entropy, enthalpy and Gibbs free energy. Arrhenius equation, transition state theory. Uses of activation parameters, Hammonds postulate. Bell-Evans-Polanyi principle. Potential energy surface model. Marcus theory of electron transfer. Reactivity and Selectivity principles

OC (CB_3) -2: Kinetic,isotopic, structural,solvent, steric and conformational effects

Theory of isotope effects, Primary and secondary kinetic isotope effects. Heavy isotope effects. Tunneling effect Solvent effects. Structural effects on reactivity: Linear free energy relationship (LFER.). The Hammett equation, substituent constants, theories of substituent effects. interpretation of σ-values. Reaction constant ρ. Deviations from Hammett equation. Dual—parameter correlations, inductive substituent constant The Taft model, σ1,σR scales. Solvation and solvent effects: Qualitative understanding of solvent- solute effects on reactivity Thermodynamic measure of solvation. Effects of solvation on reaction and equilibrium. Various empirical indexes of solvation based on physical properties, solvent- sensitive reaction rates, spectroscopic properties and scales for specific solvation. Use of solvation scales in mechanistic studies. Solvent effects from the curve-crossing model. Various type of steric strain and their influence on reactivity. Steric acceleration. Molecular measurements of steric effects upon rates. Steric LFER. Conformational barrier to bond rotation-spectroscopic detection of individual conformers. Acyclic and monocyclic systems. Rotation around partial double bonds. Winstein-Holness and Curtin-Hammet principle.

OC (CB_3) -3: Nucleophilic,electrophilic and free radical reactivity

Bases, nucleophiles, Electrophiles and Catalysts. Acid-base dissociation. Electronic and structural effects, acidity and basicity. Acidity functions and their applications. Hard and soft acids and bases. Nucleophilicity scales, Nucleofugacity. The α-effect.- Ambivalent nucleophiles. Acid-base catalysis. Specific and general catalysis. Bronstéd catalysis. .nucleophilic and electrophilic catalysis. Catalysis by non-covalent binding micellar catalysts. Nucleophilic and electrophilic Reactivity:Structural and electronic effects on SN1 and SN2 reactivity. Solvent effects,kinetic isotope effects. Intramolecular assistance. Electron transfer nature of SN2 reaction. Nuclcophilicity and SN2 reactivity based on curve-crossing model. Relationship between polar and electron transfer reactions. SRN1 mechanism. Electrophilic reactivity, general mechanism. Kinetics of SE2-Ar reaction, Structural effects on rates and selectivity. Curve crossing approach to electrophilic reactivity.

Radical and pericyclic reactivity. (a)Radical stability, polar influences, solvent and steric effects. A curve crossing approach to radical addition, factors affecting barrier heights in additions, regioselectivity in radical reactions. Reactivity, specificity and periselectivity in pericyclic reactions.

OC (CB_3) -4: Supramolecular chemistry

Properties of covalent bonds- bond length, inter-bond angles, force constant, bond and molecular dipole moments. Molecular and bond polarisability, bond dissociation enthalpy, entropy. Intermolecular forces, hydrophobic effects. Electrostatic, induction, dispersion and resonance energy, magnetic interactions, magnitude of interaction energy, forces between macroscopic bodies, medium effects, Hydrogen bond. Principles of molecular association and organization as exemplified in biological macromolecules like enzymes, nucleic acids, membranes and model systems like micelles and vesicles. Molecular receptors and design principles. Cryptands, cyclophanes, calixeranes, cyclodextxins. Supramolecular reactivity and catalysis. Molecular channels and transport processes. Molecular devices and nanotechnology.

Recommended books:

1. Molecular mechanics. By U.Bukert and N.L.Allinger, ACS Monograph 177,1982
2. Organic Chemistry book of Orbitals. L.Salem and W.L.Jorgenson
3. Mechanism and theory in Organic Chemistry, T.M.Lowry, K.C.Richardson, Harper and Row
4. Introduction to theoretical Organic Chemistry and molecular modeling by W.B.Smith, VCH,Weinhein.
5. Physical Organic chemistry, N.S.Isaaçs
6. Suprarnolecular Chemistry - concepts and perspectives by J M .Lehn,
7. The Physical basis of Organic Chemistry by H.Maskill.
8. Physical Organic Chemistry by Jack Hine

Semester IV
Laboratory courses

Paper CH (OC) 451P: Spectroscopic identification of organic compounds and Chromatography:

1. Identification of unknown organic compounds by interpretation of IR, UV, ^{1}H -NMR, ^{13}C NMR and mass spectral data. A minimum of 30 representative examples should be studied.
2. Thin layer chromatography: Determination of purity of a given sample, monitoring the progress of chemical reactions, identification of unknown organic compounds by comparing the R_f values of known standards.
3. Separation by column chromatography: Separation of a mixture of *ortho* and *para*-nitroanilines using silicagel as adsorbant and chloroform as the eluent. The column chromatography should be monitored by TLC.

Paper CH (OC) 452P: Synthesis and analysis of drugs

(A) Laboratory Synthesis of the following drugs:
Paracetamol, Phenytoin, Benzocaine, 6-Methyluracil, Chloritone,
4-Aminobenzene sulfonamide, FIuorescien and antipyrine.

(B) Estimation of the following drugs*:*
Aspirin (titrimetry), Ibuprofen (titrimetry), Analgin (titrimetry), Chloride in Ringer's lactate (argentometry), ascorbic acid {titrimetry, Iodometry and Cerimetry), colorimetry}, Isoniazid(Iodometry), Riboflavin(colorimetry),Zn ions in Bactracin Zinc,
Ca^{+2} ions in Calcium gluconate injection(complexometry), Diazepam (UV-Visible Spectrophotometer).

Recommended books:

1. Practical organic chemistry by Mann & Saunders
2. Text book of practical organic chemistry by Vogel
3. The systematic identification of organic compounds by Shriner et.al
4. Analytical chemistry by G N David Krupadanam et.al
5. Advanced practical medicinal chemistry by Ashutoshkar
6. Pharmaceutical drug analysis by Ashutoshkar
7. Quantitative analysis of drugs in pharmaceutical formulations by P D Sethi
8. Practical pharmaceutical chemistry part-1 and part-2 by A H Beekett and J B Stenlake
9. Spectroscopic identification of organic compounds by R M Silverstein and F X Webster

PHYSICAL SPECIALISATION

SYLLABUS (2012 – 13) ONWARDS

III & IV SEMESTERS

M.Sc. CHEMISTRY (PHYSICAL CHEMISTRY)

FOR STUDENTS ADMITTED IN THE YEAR (2011 – 12)

REVISED AS PER NEW (CB) SYLLABUS

M.Sc. PHYSICAL CHEMISTRY SPECIALIZATION

Syllabus for III and IV Semesters

(for the batch admitted during the academic year 2011-2012 under the CBCS pattern)

[Under Restructured CBCS Scheme]

(Approved in the P.G. BOS meeting held on 15-9-2012)

Semester - III

	Hrs/week	Internal assessment	Semester exam	Total	Credits
CH (P) 301T	4	20 marks	80 marks	100 marks	4
CH (P) 302T	4	20 marks	80 marks	100 marks	4
CH (P) 303T	4	20 marks	80 marks	100 marks	4
CH (P) 304T	4	20 marks	80 marks	100 marks	4
Seminar	2			25 marks	1
CH (P) 351P	9	_	100 marks	100 marks	4
CH (P) 352P	9	_	100 marks	100 marks	4
Total				**625 marks**	**25**

Semester - IV

	Hrs/week	Internal assessment	Semester exam	Total	Credits
CH (P) 401T	4	20 marks	80 marks	100 marks	4
CH (P) 402T	4	20 marks	80 marks	100 marks	4
CH (P) 403T	4	20 marks	80 marks	100 marks	4
CH (P) 404T (CB)	4	20 marks	80 marks	100 marks	4
Seminar	2			25 marks	1
CH (P) 451P	9	_	100 marks	100 marks	4
CH (P) 452P	9	_	100 marks	100 marks	4
Total				**625 marks**	**25**

(**Choice based paper (CB)** = Paper offered by the same Department or other Department in the Science faculty)

Grand total marks and credits (all 4 semesters) 2500 marks - 100 credits

PAPER TITLES

M.Sc. PHYSICAL CHEMISTRY SPECIALISATION

III SEMESTER SYLLABUS

(For the batch admitted during the academic year 2011-2012 under the CBCS pattern)

[Under Restructured CBCS Scheme]

PAPER-1 CH(P) 301T: CHEMICAL KINETICS, PHOTO CHEMISTRY, ELECTROCHEMISTRY & SUPRAMOLECULAR CHEMISTRY

PC-09 : Chemical Kinetics-II
PC-10 : Photochemistry-II
PC-11 : Electrochemistry -II
PC-12 : Supramolecular Chemistry

PAPER –2 CH (P) 302T : SPECTROSCOPY & LASERS

PC- 13: Physical principles of spectroscopy & Vibrational spectroscopy
PC- 14: NMR , NQR and Mossbaur Spectroscopy
PC- 15: X-ray Spectroscopy & Diffraction techniques
PC- 16: lasers in Chemistry

PAPER –3 CH(P) 303T: QUANTUM CHEMISTRY AND GROUP THEORY

PC –17: Applications of Schrödinger equation
PC - 18: Angular momentum & approximate methods
PC - 19: Bonding in molecules
PC - 20: Group theory

PAPER-4 CH(P) 304T: POLYMER CHEMISTRY

PC- 21: Polymerization & Kinetics of polymerization
PC- 22: Structure and properties of polymers
PC- 23: Processing of Polymers
PC- 24: Functional polymers

LABORATORY COURSES
Paper-V CH (P) 351 P :Chemical Kinetics)
PAPER-VI CH(P) 352P: Instrumentation

PAPER TITLES

M.Sc. PHYSICAL CHEMISTRY SPECIALISATION

IV SEMESTER SYLLABUS

(For the batch admitted during the academic year 2011-2012 under the CBCS pattern)

[Under Restructured CBCS Scheme]

PAPER-1 CH(P) 401T: THERMODYNAMICS & COMPUTATIONAL CHEMISTRY.

PC-25 : Statistical Thermodynamics

PC-26 : Non-equilibrium Thermodynamics

PC-27 : Computational Chemistry

PC-28 : Theoretical treatment of bio polymers

PAPER-2 CH(P) 402T : APPLIED CHEMISTRY AND MATERIAL SCIENCE

PC-30 : Applied Electrochemistry

PC-31 : Types of materials, conducting organics and NLO materials

PC-29 : Applied kinetics

PC-32 : Liquid crystals and nanoparticles

PAPER-3 CH(P) 403 T : CATALYSIS

PC- 33: Homogeneous catalysis

PC-34: Surface Chemistry & Micellar catalysis

PC-35: Heterogeneous catalysis

PC-36: Phase transfer , Anchored & Photo catalysis

PAPER-4 CH(P) 404T(CB_I): ENGINEERING CHEMISTRY

PC(CB_1) -1: Water and waste water treatment

PC(CB_1) -2: Corrosion and its control

PC(CB_1) -3: Energy sources:

PC(CB_1)- 4: Engineering materials.

PAPER-4 CH(P) – 404T(CB_2)T : COMPUTATIONAL CHEMISTRY & IT'S APPLICATIONS

PC(CB_2)-1: Computational Chemistry – I

PC(CB2)-2: Computational Chemistry – I

PC(CB_2)-3: Drug Design Methods I - Ligand Based

PC(CB_2)-4: Drug Design Methods II - Structure Based.

CH (P) 451P: Paper-V (Chemical Kinetics)

CH (P) 452P: Paper-VI (Instrumentation)

M.Sc. III SEMESTER
PHYSICAL CHEMISTRY Specialization
(for the batch admitted in academic year 2011 - 2012 under CBCS pattern)

PAPER-1 CH(P) 301T: CHEMICAL KINETICS, PHOTO CHEMISTRY, ELECTROCHEMISTRY & SUPRAMOLECULAR CHEMISTRY

PC-09 : Chemical Kinetics-II
PC-10 : Photochemistry-II
PC-11 : Electrochemistry -II
PC-12 : Supramolecular Chemistry

PC-09: Chemical kinetics – II: (15hrs)

Reactions in solution: Factors affecting the reaction rates in solution. Diffusion controlled reactions. Influence of dielectric constant and ionic strength on ion-ion, ion-dipole and dipole-dipole reactions. Primary and secondary salt effects. Kinetic isotope effects: Primary and secondary isotope effects. Solvent isotope effects.

Fast reactions: Flow methods and the stopped-flow technique. Relaxation methods (T-jump and P- jump). Kinetic equations for chemical relaxation.

Enzyme kinetics: Michaelis - Menten mechanisms of enzyme catalyzed reactions involving one and two intermediates. Steady-state approximation. Derivation of kinetic equations. Evaluation of kinetic parameters. Enzyme- substrate complex: Fischer's lock and key and Koshland's induced fit hypotheses. Specificity of enzyme-catalyzed reactions. Discussion of the various types of forces involved in the formation of E-S complex. pH dependence of enzyme-catalyzed reactions – the kinetics and the equations involved.

PC –10: Photochemistry – II: (15hrs)

Formation of excimers and exciplexes – PE diagram and quantum yields. Energy transfer mechanism for bimolecular quenching. Long-range coulombic energy transfer – critical transfer distance. Short-range electron exchange energy transfer. Triplet-triplet energy transfer and sensitization.

Experimental study of radiative transitions. Emission spectroscopy. Emission quenching measurements. Flash photolysis.

Organic photochemistry. Properties of (n, π^*) and (π, π^*) states.

Photochemistry of alkenes. Cis-trans isomerisation, di-π- methane rearrangement.

Photochemistry of carbonyl compounds. Norrish type-I reactions. Photoreduction. Norrish type-II reactions. Addition of carbonyl to carbon-carbon multiple bonds (Paterno-Buchi) reaction.

Barton reaction. Singlet oxygen – photooxygenation reactions .

Electronic transitions in transition metal complexes. Ligand field (LF) and charge transfer (CT) electronic states. $Ru(bpy)_3^{2+}$ as sensitizer for photoredox reactions, examples. Photochemical cleavage of water.

PC –11 : Electrochemistry – II (15 hrs)

The electrode-electrolyte interface. The electrical double layer. The Helmholtz-Perrin parallel-plate model, the Gouy-Chapman diffuse-charge model and the Stern model. Quantum aspects of charge transfer at the interfaces. Tunneling.

Electrodics. Charge transfer reactions at the electrode-electrolyte interface. Exchange current density and overpotential. Derivation of Butler-Volmer equation. High field approximation- Tafel equation, low field, equilibrium- Nernst equation. The symmetry factor and its significance.

Corrosion: Electrochemical corrosion.mechanism. short-circuited energy producing cell.

The corrosion current and the corrosion potential. Homogeneous theory of corrosion. Evans diagrams. Potential- pH (Pourbaix) diagrams of iron. Methods of corrosion rate measurement. Mechanism of anodic dissolution of iron. Corrosion inhibition by organic molecules.

PC- 12: Supra molecular Chemistry **(**15 Hrs)

Molecules, super molecules and supramolecular Chemistry.

Molecular recognition – factors involved. Ionophores. Molecular receptors – design principles. Typres of interactions between host and guest molecules.

Molecular receptors for alkali metal ions, ammonium ions, anions and neutral molecules. Crown ethers, cryptands, spherands, cyclodextrins and calixaranes.

Threading of a linear molecule through a cyclic molecule. Creation of rotaxanes and catenanes.

Thermodynamics ofhost-guest complexation. Enthalpy and entropy contributions. Complexation free energies.

Applications. Supramolecular catalysis- examples. Transport of ions across membranes. Molecular awires and molecular switches.

Books suggested:

1. Chemical Kinetics, K. J. Laidler, McGraw Hill
2. Kinetics and Mechanism, A. A. Frost & R. G. Pearson, John Wiley & sons
3. Kinetics and Mechanism of Chemical Transformations, J. Rajaraman & J. Kuriacose, McMillan
4. Chemical Kinetics and Reaction Mechanisms, J. H. Espenson, McGraw Hill
5. Physical Organic Chemistry, N. S. Isaacs, ELBS
6. The Physical basis of Organic Chemistry, Howard Maskill, Oxford University Press
7. Biophysical Chemistry, Cantor & Schimmel, W. H. Freeman and Company

8. Principles of Physical Biochemistry, Kensal E van Holde, W. Curtis Johnson & P. Shing Ho, Prentice Hall
9. Physical Biochemistry : Principles and Applications, David Sheehan, John Wiley
10. Lehninger Principles of Biochemistry, D. L. Nelson & M. M. Cox, MacMillan
11. Biochemistry, L. Stryer, W. H. Freeman and Company
12. Molecular Photochemistry, N. J. Turro, W. A. Benzamin
13. Fundamentals of Photochemistry, Rohatgi-Mukherjee, Wiley Eastern
14. Essentials of Molecular Photochemistry, A. Gilbert & J. Baggott, Blackwell Science
15. Introduction to Molecular Photochemistry, C. H. J. Wells, Chapman and Hall
16. Physical Chemistry, Ira N. Levine, McGraw Hill
17. Atkin's Physical Chemistry, P. Atkins & Julio de Paula, Oxford University Press
18. The New Chemistry, Editor-in-chief Nina Hall, Cambridge University Press
19. Modern Electrochemistry, J. O. M. Bockris & A. K. N. Reddy, Plenum
20. Introduction to Electrochemistry, S. Glasstone
21. Supramolecular Chemistry – concepts and perspectives by Jean-Marie Lehn
22. Principles and methods in supramolecular chemistry, Hans-Jorg Schneider and A.Yatsimirsky, John Wiley and Sons
23. The New Chemistry, Editor in chief : Nina Hall, Cambridge University press
24. Analytical Chemistry of Macrocyclic and Supramolecular Compounds, S.M.Khopkar, Narosa Publishing House

PAPER –2 CH (P) 302T : SPECTROSCOPY & LASERS

PC- 13: Physical principles of spectroscopy & Vibrational spectroscopy
PC- 14: NMR , NQR and Mossbaur Spectroscopy
PC- 15: X-ray Spectroscopy & Diffraction techniques
PC- 16: lasers in Chemistry

PC-13: Physical principles of spectroscopy & Vibrational spectroscopy: (15 hrs)

Interaction of electromagnetic radiation with matter. Absorption and emission of radiation. Induced absorption, spontaneous emission and stimulated emission. Einstein coefficients. Selection rules. Oscillator strength. Line width and natural line broadening. Doppler broadening. Intensity of spectral lines.
Infrared spectroscopy. Anharmonic oscillator. Morse potential energy diagram. Vibration – rotation spectroscopy, P, Q, R branches. Vibration – rotation spectra of polyatomic molecules – linear, symmetric top and asymmetric top molecules. Principles of FTIR.
Raman spectroscopy. Classical and quantum theories of Raman effect. Pure rotational, vibrational and vibrational – rotational Raman spectra. Selection rules. Depolarization factors of Raman lines and their relevance. Instrumentation. Typical applications of Raman spectroscopy.

PC-14: NMR, NQR and Mossbaur Specroscopy. (15 hrs)

Prnciple of nmr. Derivation of $h\,\nu = g\,\beta\,H$. Larmor processional frequency- spin-spin splitting (AX) - Qantitative treatment (proof for J= distance between two successive nmr spectral lines) – Instrumentation - CW and FT methods.
Two dimensional nmr spectroscopy-principles of 2D nmr-Graphical representation of 2D nmr specra – Homonuclear ^{1}H J, δ spectroscopy-its application for mixture analysis- (for instance mixture analysis of n-butyl bromide and n-butyl iodide) - The COSY experiment. Two dimensional ^{1}H, ^{1}H shift correlations. COSY spectra of an AX system, o-nitroaniline, alanine, glutamic acid and arginine. The nuclear overhauser effect(NOE). Two dimensional nuclear overhauser spectroscopy(NOSY) Applications of 2D nmr.
Nuclear Quadrupole Resonance: Quadrupole nuclei and quadrupole moments-prolate and oblate nuclear charge distributions-energies of quadrupolar transitions-electric field gradient, coupling constants and splittings
Mossbauer Spectroscopy - Mossbauer effect - typical Mossbauer spectrum - isomer shift – quadrupole splitting – magnetic hyperfine interaction – ^{57}Fe – Mossbauer spectra of Fe^{2+} and Fe^{3+} (paramagnetic) and Fe^{3+} (magnetic) compounds.

PC-15: X-ray Spectroscopy & Diffraction techniques: (15 hrs)

X-ray fluorescence (XRF) spectra : Absorption techniques, Absorption edge fine structure (AEFS spectra) and extended X-ray absorption fine structure (EXAFS) spectra.
X-ray diffraction. Bragg condition. Miller indices. Experimental methods of X-ray diffraction. Laue method and Debye-Scherrer method. Primitive and nonprimitive unit cells. Index reflections. Identification of unit cells from systematic absences in diffraction pattern. Structure factor and its relation to intensity and electron density. Description of the procedure for an X-ray structure analysis. Typical examples.

Electron diffraction. Scattering intensity versus scattering angle. Wierl equation. Measurement technique. Elucidation of structure of simple gas phase molecules.

PC 16: Lasers in Chemistry: (15 hrs)

General principles of laser action. Stimulated emission. Rates of absorption and emission. Einstein coefficients. Population inversion. Three-level and four-level laser systems. Pumping. Laser cavity – resonant modes. Characteristics of laser light. Laser pulses and their characteristics. Pulse production, Q-switching. Pulse modification, mode-locking.
Practical lasers. Solid-state lasers, gas lasers, chemical and excimer lasers. Examples.
Applications of lasers in chemistry. Femtochemistry. The pump-probe technique. Time-resolved spectroscopy. Photodissociation of ICN. Formation and dissociation of CO-hemoglobin complex. Conversion of ethylene to cyclobutane. Bond selectivity in chemical reactions – the reaction between hydrogen atoms and vibrationally excited HDO molecules.
Lasers and multiphoton spectroscopy – underlying principles. Two-photon spectra of diphenyloctatetraene. Lasers in fluorescence spectroscopy and Raman spectroscopy.

Books suggested:

1. Modern Spectroscopy, J. M. Hollas, John Wiley & sons
2. Fundamentals of Molecular Spectroscopy, Banwell & McCash
3. Introduction to Molecular Spectroscopy, G. M. Barrow, McGraw Hill
4. Molecular Spectroscopy, J. D. Graybeal, McGraw Hill
5. Basic principles of Spectroscopy, R. Chang, McGraw Hill
6. Physical Methods in Chemistry, R. S. Drago, Saunders College
7. Vibrational Spectroscopy: Theory and Applications, D. N. Sathyanarayana, New Age International
8. Introduction to Raman Spectroscopy, J. R. Ferraro & K. Nakamoto, Academic Press
9. NMR Spectroscopy: Basic principles, concepts and applications in chemistry, H. Gunther, John Wiley & sons
10. Introduction to Magnetic Resonance, A. Carrington & A.D. Maclachalan, Harper & Row

11. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R. V. Parish, Ellis Harwood
12. NMR basic principles - Atta-ur-Rahman
13. Two dimensional NMR Spectroscopy-Applications for chemists and biochemists, edited by W. R. Croasmun & R. M. K. Carlson, VCH
14. X-ray diffraction procedures for polycrysralline and amorphous materials, H. P. Klug & L. E. Alexander, John Wiley
15. Physical Chemistry, Ira N. Levine, McGraw Hill
16. Atkin's Physical Chemistry, P. Atkins & Julio de Paula, Oxford University Press
17. A Guide to Lasers in Chemistry, G. R. Van Hecke & K. K. Karukstis, Jones and Bartlett Publishers
18. Lasers in Chemical and Biological Sciences, S. Chopra & H. M. Chawla, Wiley Eastern Ltd

PAPER –3 CH(P) 303T: QUANTUM CHEMISTRY AND GROUP THEORY

PC –17: Applications of Schrödinger equation
PC - 18: Angular momentum & approximate methods
PC - 19: Bonding in molecules
PC - 20: Group theory

PC – 17 : Applications of Schrödinger equation (15 hrs)

Systems with discontinuity in the potential field. A simple potential barrier. A potential barrier with a finite thickness. Quantum mechanical tunneling – examples - α-particle emission, inversion of NH_3, hydrogen transfer reactions.
The harmonic oscillator – detailed treatment. Wave functions and energies. Vibration of a diatomic molecule – harmonic oscillator model.
The rigid rotator – detailed treatment. Wave functions and energies. Spherical harmonics. Rigid rotator as model for a rotating diatomic molecule.
The hydrogen atom – detailed treatment. Angular and radial functions. Atomic orbitals. Measurability of the ground-state energy of hydrogen atom. Orthonormal nature of hydrogen-like wave functions. Probability calculations.
Atoms in external field, Zeeman and anomalous Zeeman effect.

PC – 18: Angular momentum & approximate methods (15 hrs)

Angular momentum operators. Commutation relations of angular momentum operators and their consequence. Eigen functions of L^2 and L_z and the eigen values. Magnitude and orientation of angular momentum vectors.
Electron spin. Spin operators. Pauli principle and the Pauli exclusion principle.
Approximate methods. The variation method. Constuction of variation function by the method of linear combinations. H and He atom.
Perturbation theory (first order and nondegenerate). Wave function and energy corrections. Application of perturbation theory to the helium atom.
Time- dependent perturbation theory. Interaction of radiation and matter. Allowed and forbidden transitions.
Multielectron atoms. The Hartree-Fock self-consistent field method. Basis functions. Slater-type orbitals (STOs).

PC – 19: Bonding in molecules (15 hrs)

Born-Oppenheimer approximation. MO theory of H_2^+ ion. Calculation of MOs and their energies. Evaluation of the overlap integral. Probability curves and enegy diagram. MO theory of H_2 molecule. Calculation of energy. Atomic and molecular term symbols.MO theory of polyatomic molecules (general ideas). MO treatment of H_2O. Symmetry-adapted linear combinations. MOs of H_2O.
Concept of hybridization – sp, sp^2, and sp^3 hybrid orbitals.

Semiempirical MO methods. The Huckel theory of conjugated systems. HMO calculations on ethylene, allyl system, butadiene, cyclopropenyl system and benzene. π–electron charges and bond orders. Introduction to extended Huckel theory.
Orbital symmetry and reactivity: $H_2 + F_2 \rightarrow 2HF$ reaction. 2NO $N_2 + O_2$ reaction. Electrocyclic reactions, cycloaddition reactions.

PC – 20: Group theory (15 hrs)

Matrices: Addition and multiplication of matrices. Diagonal matrix. Unit matrix. Transpose of a matrix. Adjoint of a matrix. Inverse of a matrix. The determinant of a square matrix. Expansion of a determinant. Properties of determinants
Symmetry operations forming a group. Classes of symmetry operations. Matrix representation of symmetry operations and point groups. Generation of representations for point groups. Reducible and irreducible representations.
The Great Orthogonality theorem (proof not required) and its consequences. Relation between reducible and irreducible representations. Character tables. Construction of character tables for C_{2v} and C_{3v} groups.
Quantum mechanics and group theory. Wave functions as bases for irreducible representations. The direct product – vanishing of integrals. Projection operators. Symmetries of vibrations. IR and Raman activity.

Books suggested:

1. Quantum Chemistry, Ira N. Levine, Prentice Hall
2. Introduction to Quantum Chemistry, A. K. Chandra, Tata McGraw Hill
3. Elementary Quantum Chemistry, F. L. Pilar, McGraw Hill
4. Molecular Quantum Mechanics, P. W. Atkins & R. S. Friedman, Oxford University Press
5. Coulson's Valence, R. McWeeny, ELBS
6. The Chemical Bond, J. N. Murrel, S. F. A. Kettle & J. M. Tedder, John Wiley
7. Valency Theory, J. N. Murrel, S. F. A. Kettle & J. M. Tedder, ELBS
8. Chemical Applications of Group Theory, F. A. Cotton, John Wiley & Sons

PAPER-4 CH(P) 304T: POLYMER CHEMISTRY

PC- 21: Polymerization & Kinetics of polymerization
PC- 22: Structure and properties of polymers
PC- 23: Processing of Polymers
PC- 24: Functional polymers

PC -21: Polymerization & Kinetics of polymerization (15 hrs)

Classification of polymers. Types of polymerization. Kinetics and mechanism of free radical polymerization. Degree of polymerization, kinetic chain length and chain transfer coefficient – Trommsdorff effect. Effect of pressure and temperature on chain polymerization.

Kinetics and mechanism of linear stepwise polymerization, cationic, anionic polymerization. Coordination polymerization. copolymerization reactions and copolymer composition. Reactivity ratios and their determination. Alfrey and Price Q-e scheme for monomer and radical reactivity. Block and graft copolymers.

Polymerization in homogeneous and heterogeneous systems. Bulk, solution, suspension and emulsion polymerizations.

PC -22:Structure and properties of polymers (15 hrs)

Polymer solutions. The process of polymer dissolution. Thermodynamics of polymer dissolution. Entropy, heat and free energy of mixing of polymer solutions. Conformations of dissolved polymer chains. The freely jointed chain. Short-range and long-range interactions. The Flory-Huggins theory of polymer solutions. Dilute polymer solutions. Flory-Krigbaum theory.

Mechanical properties of polymers. The elastic state. Rubber-like elasticity and viscoelasticity. Newtonian and non-Newtonian behaviour. Maxwell and Voigt-Kelvin models of viscoelastic behaviour.
The crystal structure of polymers. Morphology of crystalline polymers. Crystallization and melting. Determination of T_m. Thermodynamics of crystalline melting. Heats and entropies of fusion. Degree of crystallinity. Factors affecting the crystallization. The glassy state – glass transition temperature T_g of polymers. Factors influencing T_g. Glass transition temperature and melting point. Molecular weight distribution – measurement of molecular weights by end group analysis, osmometry and GPC

PC -23: Processing of Polymers (15hrs)

General Applications of Polymers. Polymer Processing - Fillers, Additives, Lubricants, Catalysts, Colorants, Lamination, Adhesives , Calendering and Composites.
Moulding of Polymers- Process and Advantages and limitations of Compression moulding, Injection Moulding, Extrusion Moulding, Blow Moulding.
Casting- Types, Vacuum Casting, Potting, Encapsulation, Film Casting, Pultrusion technique.
Fibre Reinforced Plastics, preparation and properties.
Synthetic Fibres- Rayons, (Nitro cellular, Cupammonium, Diacetate, Viscose), Nylons, Dacron, Dry & Wet methods of fibre formation. Mercerization

PC -24: Functional Polymers (15hrs)

Smart materials – their uses in sensing devices and communication networks.
Conducting polymers. Electrically conducting polymers and their uses (polyanilines, polypyrrole, polyacetylene and polythiophene). Photoconductive polymers. Liquid crystal polymers – smectic, nematic and cholesteric structures.
Ionic exchange polymers. Cationic and anionic exchange polymers and their uses. Eco-friendly polymers.
Membrane separation. Filtration – micro, ultra and nanofiltration. Separation of gases – permeselectivity and gas permeability of representative polymers. Liquid separation – dialysis, electro osmosis and reverse osmosis. Fire retarding polymers, photonic polymers.
Polymers in biomedical applications – artificial organs and controlled drug delivery.

Books suggested:

1. Textbook of Polymer Science, F. W. Billmeyer Jr, John Wiley & sons
2. Polymer Science, V. R. Gowarikar, N. V. Viswanathan & J. Sreedhar, Wiley Eastern
3. Contemporary Polymer Chemistry, H. R. Alcock & F. W. Lambe, Prentice Hall
4. Physics and Chemistry of Polymers, J. M. G. Cowie, Blackie Academic and professional
5. Ploymer Chemistry, B. Vollmert
6. Physical Chemistry of Polymers, A. Tagers, Mir Publishers
7. A text book of polymers, Vol. I,II,III, M.S. Bhatnagar , S. Chand

PRACTICALS- III SEMESTER:

CH (P) 351 P: Paper-V (Chemical Kinetics) 9 hrs/ week

Note: The data obtained in all the experiments are to be analyzed by the students both *by the usual graphical methods and by regression (linear/nonlinear) techniques using a PC.*

- Study of peroxydisulphate – iodide reaction:
  - Individual orders of the reactants by initial rate methods
  - Effect of temperature on reaction rate
  - Effect of ionic strength on reaction rate
- Study of peroxydisulphate – iodide clock reaction: Individual orders of the reactants ,effect of ionic strength on uncatalyzed and Cu(II)-catalyzed reactions
- Study of acetone – iodine reaction by titrimetry
  - Order w.r.t.[iodine]
  - Order w.r.t. [acetone]
  - Order w.r.t. $[H^+]$

CH (P) 352 : Paper-VI (Instrumentation) 9 hrs/ week

Conductometry:

- Conductometric titrations:
  - Mixture of strong and weak bases vs strong acid
  - Mixture of strong and weak acids vs weak base
  - Mixture of strong acid, weak acid and $CuSO_4$ vs strong base
  - Mixture of halides (chloride + iodide) vs $AgNO_3$
  - Formic acid, acetic acid, chloroacetic acid, dichloroacetic acid and Trichloroacetic acid and their mixtures vs strong base
  - Precipitation titration: K_2SO_4 vs $BaCl_2$
- Dissociation constants of weak acids
- Effect of solvent on dissociation constant of a weak acid
- Verification of Onsager equation
- Composition of Cu(II) – tartaric acid complex by Job's method

pH metry:

- pH – metric titrations:

Monobasic acids vs strong base
Dibasic acid vs strong base
Tribasic acid vs strong base
Mixture of strong and weak acids vs strong base

- Determination of dissociation constants of monobasic/dibasic acids by Albert – Serjeant method
- Determination of dissociation constant of acetic acid in DMSO, acetone and dioxane
- Determination of pK_a and pK_b of glycine (calculation using a computer program)
- Determination of stability constant of a metal complex (calculation using a

M.Sc. IV SEMESTER
PHYSICAL CHEMISTRY Specialization
(for the batch admitted in the academic year 2010-2011 under CBCS pattern)

PAPER-1 CH(P) 401T: THERMODYNAMICS & COMPUTATIONAL CHEMISTRY.

PC-25 : Statistical Thermodynamics
PC-26 : Non-equilibrium Thermodynamics
PC-27 : Computational Chemistry
PC-28 : Theoretical treatment of bio polymers

PC -25: Statistical Thermodynamics (15 hrs)

Concepts of distribution and probability. Estimation of probability and the most probable distribution. Systems composed of noninteracting particles. Derivation of Boltzmann distribution law.

The molecular partition function. Systems composed of interacting particles. The concept of ensemble and canonical ensemble. Canonical partition function and its relation to molecular partition function. The factorization of molecular partition function – translational, rotational, vibrational and electronic partition functions. Derivation of expressions for translational, rotational (diatomic) and vibrational partition functions. Relationship between partition functions and thermodynamic functions.

The relationship between partition functions and thermodynamic functions. Law of equipartition energy.

Specific heats of solids – Einstein equation of heat capacity of solids – derivation. Explanation of heat capacity at very low and very high temperatures – Dulong and Petits Law. Debye theory.

The entropy of a monoatomic ideal gas. The Sackur-Tetrode equation- derivation. Mean translational and vibrational energies.

The relation between equilibrium constant and partition function- derivation.

Basic ideas of Bose-Einstein statistics and Fermi-Dirac statistics and comparison of these with Maxwell-Boltzmann statistics.

PC - 26. Non-equilibrium Thermodynamics (15hrs)

Thermodynamic criteria for non-equilibrium states. Entropy production in irreversible processes. Entropy production in heat flow and entropy production in material flow. Fluxes and forces. Linear flux-force relations**.** Phenomenonological equations and coefficients. Microscopic

reversibility. Onsager reciprocal relations (proof not required). Application of Onsager relations to electrokinetic phenomena – electroosmotic pressure and streaming current. The Onsager relations and the principle of detailed balance. Liquid junction potentials – derivation of equation for liquid junction potential in terms of transport numbers using Onsager relations.Steady states. Principle of minimum entropy production. Irreversible thermodynamics as applied to biological systems – examples – sodium potassium pump, gulucose transport. Application to thermoelectric circuits. Seebeck and Peltier effect.

PC-27: Computational treatement of many electron systems (15hrs)

Multi-electron atoms. The antisymmetry principle and the Slater determinant. The Hartree-Fock method. The Hartree-Fock equations.(no derivation). The Fock operator. Core hamiltonian. Coulomb operator and exchange operator. Slater-type orbitals (STOs) as basis functions. Orbital energies and total energy. Helium atom example. Koopman's theorem. Hund's rules and theoretical basis of the Aufbau principle. Electron correlation energy.The Hartree-Fock method for molecules. Restricted and unrestricted HF calculations. The Roothan equations. The Fock matrix. The Roothan matrix elements. GTOs and different types of basis sets. Minimal basis set. Model HF calculations on H_2. Discussion of results of HF calculations on simple molecules – H_2O and NH_3. Introduction to configuration interaction.Density functional theory (DFT). Hohenberg-Kohn theorem. Kohn-Sham (KS) formulation of DFT. KS equations and KS orbitals. Brief explanation of exchange-correlation energy and exchange- correlation potential.

PC -28: Theoretical treatment of biopolymers (15 hrs)

Biolpolymer interactions. Basic principles of molecular mechanics. Molecular potentials. Bonding and nonbonding potentials. Electrostatic interactions, dipole-dipole interactions and van der Waals interactions. Hydrogen bonds.

Protein structure. Stabilizing interactions in proteins. The Corey-Pauling rules. The α-helix and the β-sheet. Conformational energy. Potential energy diagrams and Ramachandran plots.

Chain configuration of macromolecules. Random linear structure of biopolymers. Random walk. Random coils and measures of size – the contour length, the rms separation and the radius of gyration. Conformational entropy. Introductory treatment of the protein folding problem.

Books suggested:

1. Elements of Statistical Thermodynamics, L. K. Nash, Addison – Wesley
2. Introduction to Statistical Thermodynamics, T. L. Hill, Addison Wiley
3. Statistical Thermodynamics, M. C. Gupta, New Age International
4. Atkin's Physical Chemistry, P. Atkins & Julio de Paula, Oxford University Press
5. Molecular Thermodynamics, D. A. McQuarrie & J. D. Simon, University Science Books
6. Quantum Chemistry, I. N. Levine, Prentice Hall

7. Molecular Quantum Mechanics, P. W. Atkins and R. S. Friedman, Oxford University Press
8. Introduction to Computational Chemistry, F. Jensen, John Wiley & Sons
9. Elementary Quantum Chemistry, F. L. Pilar, McGraw Hill
10. Modern Quantum Chemistry, A. Szabo and N. S. Ostlund, Dover
11. Computational Chemistry: Introduction to the theory and Applications of Molecular and Quantum Mechanics, Errol Lewars, Springer Publications
12. Physical Chemistry, D. A. McQuarrie and J. D. Simon, Viva Books Ltd.
13. Approximate Molecular Theory, J. A. Pople and D. L. Beveridge, McGraw Hill
14. Biophysical Chemistry, Cantor & Schimmel, W. H. Freeman and Company
15. Principles of Physical Biochemistry, Kensal E van Holde, W. Curtis Johnson & P. Shing Ho, Prentice Hall
16. Physical Biochemistry : Principles and Applications, David Sheehan, John Wiley
17. Physical Chemistry for the Chemical and Biological Sciences, Raymond Chang, University Science Books
18. Biochemistry, L.Stryer, W.H. Freeman and Company

PAPER-2 CH(P) 402T : APPLIED CHEMISTRY AND MATERIAL SCIENCE

PC-30 : Applied Electrochemistry
PC-31 : Types of materials, conducting organics and NLO materials
PC-29 : Applied kinetics
PC-32 : Liquid crystals and nanoparticles

PC-29:Applied kinetics (15 hrs)

Kinetics and chemical reaction engineering.
Reactor design: Basic objectives in design of a reactor. Parameters affecting the reactor performance. Balance equations for reactor design. Single ideal reactor models.
Batch reactors (BR). General features. Design equations for a BR. Material and energy balances. Isothermal operation, constant-density system.
*Continuous stirred-tank reactors (CSTR***)**: General features. Design equations for a CSTR. Material and energy balances. Constant-density system. Steady-state operation at specified temperature.
Plug-flow reactors (PFR): General features. Design equations for a PFR. Material and energy balances. Constant-density system.
Comparisons of ideal reactors for a single reaction. Single-vessel comparisons. BR and CSTR. BR and PFR. Numerical examples.

PC -30 : Applied Electrochemistry (15 hrs)

Batteries. Battery parameters. Energy density and power density. Measures of battery performance. Primary and secondary batteries. Zn/MnO_2, lead-acid and Ni-Cd batteries. Zinc-air and lithium batteries.
Fuel cells. Types of fuel cells : H_2/O_2 and methanol/O_2, Phosphoric acid, High-temperature fuel cells. Use of porous electrodes in fuel cells.Advantages and limitations of fuel cells. Photovoltaic cells. Semiconductor based photoelectrochemical cells. Electrochemical energy from solar energy.
Anodic oxidation of metals. Characteristics of anodic oxide films. Industrial application of anodic oxide films. Electroplating, technical importance. Mechanism of electroplating. Alkaline and acid plating of copper., nickel .
Electro-organic synthesis. Reduction of carboxylic acids, the polymerization of acrylonitrile to adiponitriles in the synthesis of nylon – Reduction of nitro compounds.

PC -31: Types of materials, Conducting Organics and NLO materials (15 hrs)

Classification of materials – metals, ceramics, polymers, composites, semiconductors and biomaterials.

Glassy state – glass formers and glass modifiers, applications

Ceramics – criteria for determining the crystal structure of ceramic materials – examples. Mechanical properties of ceramics.

Composites – particle reinforced and fibre reinforced composites.

Preparative methods of solid materials. Ceramic method – coprecipitation, sol-gel, high pressure and hydrothermal methods – Arc technique.

Techniques of single crystal growth – growth from solutions – growth from melts – growth from vapour.

NLO materials – basic concepts, second and third harmonic generation, examples of organic, inorganic and polymer nlo materials.

Conducting organics – Fullerenes, alkali metal doped fullerides, fullerenes as superconductors

PC-32: Nanoparticles and their applications 15hrs

Introduction to nano particles. Preparation of nano particles –various methods- RF plasma, chemical methods, thermolysis, pulsed laser methods, optical and electrical properties of nanoparticles. Characterization of nano particles-experimental methods-powder X-ray diffraction, transmission electron microscopy (TEM), scanning electron microscopy (SEM) and atomic force microscopy(AFM).

Reduced dimensionality in solids – zero dimensional systems, fullerenes, quantum dots. Optical properties of quantum dots. One dimensional systems, carbon nano tubes, electric, mechanical and other properties.

Applications of nano particles in – photocatalysis, laser and light emitting diodes, optical filters, optical band gap materials. Use of carbon nano tubes in fuel cells and catalysis.

Books suggested:

1. Introduction to Chemical reaction Engineering and Kinetics, R. W. Missen, C. A. Mims & B. A. Saville, John Wiley
2. Chemical Reaction Engineering, O. Levenspiel, John Wiley
3. Chemical Engineering Kinetics, J. M. Smith, McGraw Hill
4. Elements of Chemical Reaction Engineering, H. Scott Fogler, Prentice Hall
5. Modern Electrochemistry 2B, Bockris & Reddy, Plenum
6. J. Chem. Educ. Vol 60, no 10,1983
7. Industrial Electrochemistry, D. Pletcher, Chapman & Hall
8. Introduction to Electrochemistry, S. Glasstone
9. Fundamental principles of Modern Electroplating, Lowenheim, John Wiley
10. The physics and chemistry of solids. Stephen Elliot, John Wiley & Sons

11. Introduction to nanotechnology.Charles P.Poole Jr, F.J.Owens,Wiley India Pvt. Ltd
12. Solid state chemistry and applications. A.R.West
13. New directions in solid state chemistry. CNR Rao and Gopalakrishnan
14. Principles of the Solid State, H. V. Keer, New Age International
15. Material Science and Engineering – An Introduction, William D. Callister, Jr., John Wiley & Sons
16. Materials Science & Engineering – A First Course, V. Raghavan, Prentice Hall
17. Nanostructured Materials and Nanotechnology, edited by Hari Singh Nalwa, Academic Press
18. Self Assembled Nanostructures, Jin Zhang, Zhong-lin Wang, Jun Liu, Shaowei Chen & Gang-Yu-Liu, Kluwer Academic/Plenum

PAPER-3 CH(P) 403 T : CATALYSIS

PC- 33: Homogeneous catalysis
PC-34: Surface Chemistry & Micellar catalysis
PC-35: Heterogeneous catalysis
PC-36: Phase transfer , Anchored & Photo catalysis

PC- 33: Homogeneous catalysis. (15 hrs)

Introduction to catalysis. Types of catalysis, characteristics of catalyst, catalyst supports, promoters, general mechanism of catalysis, equilibrium treatment and steady state treatment. Activation energies of catalyzed reactions. Acid-base catalysis, general acid base catalysis, mechanism of acid –base catalysis, catalytic activity and acid-base strength- Bronsted relationships.

Acidity functions: The Hammett acidity function. Measurement of Hammett acidity function(Ho), usefulness of Hammett acidity function in understanding the mechanism of an acid catalyzed reactions. Zucker-Hammett hypothesis and the Bunnett's theory.

Catalysis by transition metal ions and their complexes. Use of Ziegler –Natta and metallocene catalysts as homogeneous catalysts for polymerization of olefins. Some industrially important catalytic processes. The Waker process, the hydrogenation of alkenes.

PC- 34: Surface Chemistry & Micellar catalysis (15hrs)

Surface tension. Curved interfaces. The Laplace equation. Capillary action. Thermodynamics of surface layers – Gibbs isotherm.
Adsorption. Types of adsorption, factors effecting adsorption, determination of heats and entropies of adsorption. Surface versus bulk structures. Adsorbate -induced restructuring of surfaces. Thermal activation of bond breaking on a surface. Co-adsorption. Chemisorption isotherms. Kinetics of chemisorption. Surface films. Monometellic surfaces and bimetallic surfaces. Experimental techniques for the study of monolayer films. States and reaction in monomolecular films. Reaction between $H_2(g)$ and $N_2(g)$ catalyzed by surfaces to give $NH_3(g)$.
Solid-liquid boundary- charged interface, electrokinetic phenomena. Streaming current, streaming potential, electro osmosis and electro osmotic pressure – electrical double layer and explanation of these phenomena. The zeta potential and its determination. Sedimentation potential.
Micelles: Classification of surface active agents .Micellization and micellar interactions, Structure of micelles – spherical and laminar**.** Critical micellar concentration (CMC). Factors affecting the CMC of surfactants. Counter ion binding to micelles. Thermodynamics of micellization. Phase separation and mass action models, solubilization, micro emulsion, reverse

micelles reactions assisted by micelle formation. Examples of micelle-catalyzed reactions and their mechanisms.

PC- 35: Heterogeneous catalysis. (15 hrs)

Heterogeneous catalysis. Broad categories of catalysts – metals, bimetals, semiconductors, insulators, zeolites, oxides, nano materials.
Preparation of metal catalysts , supported metal catalysts and non- metallic catalysts
Characterization of catalysts: Surface area by BET method. Determination of pore volume and pore size distribution by BJH method. Pore size and specificity of catalysts. Surface acidity of catalysts- Determination of surface acidity by indicator method , IR spectroscopic method and TPD methods. Steps in heterogeneous catalyzed reactions. Diffusion and adsorption. Mechanism of surface-catalyzed reactions. The Langmuir-Hinshelwood and the Eley-Rideal mechanism. Rate constants and activation energies of surface reactions. Catalytic activity – the determining factors. Cracking and reforming, auto exhaust emissions- catalytic converters. Catalytic hydrogenation and oxidation reactions. Cracking and reforming. Fischer-Tropsch synthesis of methanol. Structure sensitive and structure insensitive catalyats. Autoexhaust emissions-catalytic converters.

PC- 36: Phase transfer, Anchored & Photo catalysis **(**15 hrs)

Phase-transfer catalysis (PTC): Principles of phase-transfer catalysis. PTC classification. Role of water in phase-transfer catalyzed reactions. Factors influencing the rate of PTC reactions. Inverse phase transfer catalysis. Mechanism of nucleophilic displacement reactions. Crown ethers. Crown ethers as PTCs in the reaction of alkyle halides with super oxide. Permanganate oxidation of alkenes and phenols in the presence of quarternary ammonium salts and crown ethers as PTCs
Anchored catalysis: Definition and examples of anchored catalysis- organic polymers, inorganic oxides and clays as supports. Structure of montmorillonite anchored catalysts- HEW structure and EF structure. Montmorillonite anchored catalysts- Application of intercalated clay catalysts- application of intercalated clay catalysts in hydrogenation reactions.

Photo catalysis: Photocatalytic effect, metal semiconductor systems as photo catalysts, nature of the metal loaded, extent of metal loading, nature of semiconductor, doped semiconductors, coupled Semiconductors. Application of photocatalysis for splitting of water by semiconductor particles, removal of organic and inorganic pollutants, for oxidation and reduction of organic compounds.

1. Principles of Heterogeneous Catalysis in practice, G. C. Bond, Oxford Publishing
2. Heterogeneous Catalysis, C. Satterfield, McGraw Hill
3. Catalysis, Principles and applications, edited by B. Vishwanathan, S. Sivasanker & A. V. Rama Swamy, Narosa Publishing House
4. Catalysis, J. C. Kuriacose, Macmillan

5. Colloidal and surface chemistry , M. Satake, Y. Hayashi, Y.Mido, S.A.Iqbal and M.S.sethi
6. Physical Organic Chemistry by L.P.Hammett, chapter 9 , McGraw Hill .
7. Chemical Review, 57**,** 1935(1957), M.A. Paul and F.A. Long
8. Phase Transfer Catalysis, Fundamentals, Applications and Industrial perspective, C. M. Stark, C. Liotta & M. Halpern, Academic Press
9. Phase Transfer Catalysis, E. V. Dehmlow & S. S. Dehmlow, Verlag Chemie, Weinheim
10. Phase Transfer Catalysis in Organic synthesis, W. P. Weber & G. W. Gokel, Springer
11. Hand book of phase transfer catalysisEdited by Y. Sasson and R. Neumann
12. Catalysis in Micellar and Macromolecular systems, J. H. Feudler & E. J. Feudler, Academic Press
13. Reaction Kinetics in Micelles, E. H. Codes (ed), Plenum
14. Micelles – Theoretical and Applied aspets, V.Moroi, plenum
15. Physical Chemistry of surfaces, A.W.Adamson and A.P.gast, Wiley
16. Polymer supported Catalysts, C. U. Pittman Jr, vol 8, Comprensive Organometallic Chemistry

CHOICE BASED (CB) PAPERS:

PAPER-4 CH(P) 404T(CB_I): ENGINEERING CHEMISTRY

PC(CB_1) -1: Water and waste water treatment
PC(CB_1) -2: Corrosion and its control
PC(CB_1) -3: Energy sources:
PC(CB_1)- 4: Engineering materials.

PC(CB_1)-1: Water and waste water treatment (15 hrs)

Review of Hardness: causes, measurement of hardness, units- types of hardness, estimation of temporary and permanent hardness, numerical problems. Boiler troubles- scales and sludge formation, caustic embrittlement, priming and foaming. Methods for boiler water treatment: Soda-lime process, zeolite process, ion exchange process. Treating saline water: distillation, electrodialysis, reverse osmosis. Municipal water supply: sedimentation, filtration, sterilization. Waste water treatment: physical, chemical and biological treatment. Sewage water , COD and BOD , numerical problems

PC(CB_1)-2: Corrosion and its control: (15 hrs)

Magnitude of the problem, theories of corrosion, Chemical and electrochemical corrosion, corrosion reactions, Types of corrosion : Galvanic, Concentration cell, soil, pitting, water line, stress, microbiological, erosion corrosions.

Factors influencing corrosion- nature of metal, purity of metal,electrochemical series, over voltage, nature of oxide film, nature of corrosion product, cathodic and anodic areas, effect of temperature, effect of pH, effect of oxidant.

Corrosion control methods- design and material selection, cathodic protection: sacrificial anode, impressed current cathode.

Protective coatings: Surface preparation, metallic coatings: hot dipping, galvanizing, tinning, cladding, electroplating, chemical conversion coatings. Chemical conversion coatings: phosphate, chromate, chemical oxide coatings, anodized coatings. Organic surface coatings-paints, constituents of paints and their functions, varnishes, enamels, lacquers.

PC(CB_1)-3: Energy sources: (15 hrs)

Conventional energy resources: Chemical fuels, classification, (solids, liquids, gaseous) . Solid fuels: coal, analysis of coal , proximate and ultimate analysis and their significance. Liquid fuels: petroleum, refining of petroleum, cracking , reforming. Synthetic petrol- Bergius and Fischer-Tropsch's process, knocking, anti knocking agents, octane number. Diesel fuel: Cetane number. Other liquid fuels: LPG, biodiesel, kerosene, fuel oil, benzol, tar, power alcohol. Gaseous fuels: natural gas, coal gas, producer gas, oil gas, water gas, biogas, Combustion: Calorific value and its determination, bomb calorimeter. HCV and LCV values of fuels, problems. analysis of flue gas

by Orsats method. Rocket fuels, solid propellants, liquid propellants, monopropellants, bipropellants

Non conventional energy resources: Nuclear fuels- nuclear reactor, nuclear fission, nuclear fusion, sources of nuclear fuels, disposal of radio active wastes, reprocessing of nuclear fuels. solar, hydro, wind, tidal energies. Bio fuels, H_2 as a non polluting fuel.

PC(CB_1)-4: Engineering materials. (15 hrs)

***Cement*:** composition of Portland cement, analysis, setting and hardening of Portland cement (reactions), decay of cement concrete, lime, manufacture, types of lime, plaster of paris

Lubricants: Criterion of a good lubricant, classification of lubricants: petroleum oils, fixed oils, synthetic lubricants, semisolid lubricants, solid lubricants. Properties of lubricants: cloud point, pour point, flash and fire point, viscocity.

Refractories: Classification, characteristics of good refractory, failure of refractories. Glass, glass making oxides and their functions, manufacture of glass. Porcelain, enamels, abrasives.

Conductors and insulators: Classification of insulators, characteristics of thermal and electrical insulators and super conductors (Nb-Sn alloy, $YBa_2Cu_3O_{7-x}$) applications.

Composite materials: Advantageous properties of the composites, classification, mechanism of strengthening, mechanism of hardening of particle reinforcement, fabrication of the composites.

Liquid crystals: Characteristics of liquid crystal orders, physical properties of liquid crystals, classification of Liquid crystals, types of mesophases chemical nature of Liquid crystals, applications of Liquid crystals, future of liquid crystals.

Reference books:

1. Text book of Engineering Chemistry by C.P. Murthy, C.V. Agarwal & A. Naidu: B.S. Publications, Hyderabad (2006).
2. Text book of Engineering Chemistry by S.S. Dara: S. Chand & Co. New Delhi (2006).
3. Engineering Chemistry by B. Siva Shanker : Mc-Graw Hill publishing Company Limited, New Delhi (2006)
4. Engineering Chemistry by J.C. Kuriocose & J. Rajaram: Tata McGraw Hill Co. New Delhi (2004)
5. Engineering Chemistry by P.C. Jain & Monica Jain, Dhanpatrai publishing company,(2008)
6. Chemistry of Engineering Materials by C.V. Agarwal, C.P. Murthy & A. Naidu: BS publications
7. Chemistry of Engineering Materials by R.P. Mani & K.N. Mishra, CENGAGE learning
8. Applied Chemistry – A text book of engineering and Technology – Springar (2005)
9. Text book of Engineering Chemistry by Shasi Chawla: Dhanpatrai Publishing company, New Delhi (2008)
10. Engineering Chemistry by R. Gopalan, D. Venkatappayya & D.V. Sulochana Nagarajan – Vikas Publishers (2008).

PAPER-4 CH(P) – 404T(CB_2) : COMPUTATIONAL CHEMISTRY & IT'S APPLICATIONS

PC(CB_2)-1: Computational Chemistry – I
PC(CB2)-2: Computational Chemistry – I
PC(CB_2)-3: Drug Design Methods I - Ligand Based
PC(CB_2)-4: Drug Design Methods II - Structure Based.

PC(CB_2)-1: Computational Chemistry – I (15hrs)

Introduction to Molecular Modeling, Single molecule calculations, assemblies of molecules and reactions of molecules - Co-ordinate systems, Cartisian and internal Co ordinates, Z- matrix, Potential energy surface - Conformational search - Global minimum, Local minima, Conformational analysis of ethane.

Force field - Features of Molecular Mechanics –Bonded and Non bonded interactions. Bond Stretching – Angle Bending, Torsional Terms – Improper Torsions and out of Plane Bending Motions – Cross Terms. Non Bonded Interactions – Electrostatic Interactions - Van-der Waals interactions - Hydrogen Bonding, Miscellaneous interactions.

PC(CB_2)-2: Computational Chemistry - II (15hrs)

Force Field Equation in Energy minimization (Energy as function of r, θ, ω) and variation w.r.t ω only - Introduction to Derivative Minimization Methods – First Order Minimization – The steepest Descent Method – Conjugate Gradients Minimization – Conformational Search procedures - Geometry optimization procedures - Introduction to molecular dynamics– description of molecular dynamics- basic elements of monte carlo method-differences between molecular dynamics and monte carlo method. Qualitative (brief) exposure to molecular dynamics simulations, conformational analysis.

PC(CB_2)-3: Drug Design Methods I - Ligand Based (15hrs)

Lead Molecule - Structure Activity Relationship (SAR) –QSAR- Physicochemical parameters, Hydrophobicity, Electronic effects, Steric Factors: Molar refractivity, Verloop steric factor and other physicochemical parameters .
Methods used in QSAR studies- Correlation of Biological activity with physico chemical Parameters – Multivariate Statistics, Partial Least Squares Method - Correlation – Regression –

Principal Component Analysis - Cluster significant analysis - Application of Hammet equation, Hansch analysis, significance of slopes and intercepts in Hansch analysis. QSAR- 2D
Linear Free Energy Relationship (LFER) - Craig plot - Topliss scheme - Bioisosteres - ree-Wilson approach - Molecular Descriptor analysis - Structure representation – QSAR 3D, CoMF A, CoMSIA.

PC(CB_2)-4: Drug Design Methods II - Structure Based. (15hrs)

Database similarity searches - Pair-wise alignment - Dot matrix comparison Needleman - Wunsch Global sequence analysis - Smith waterman Local Sequence Alignment - Multiple Sequence Alignment - Homology Modeling - Energy minimization methods - Active site Identification - Virtual Screening - Small molecule Building - Docking Algorithms - Docking Analysis. De novo Ligand design.

References:

1. Molecular Modelling: Principles and Applications, by Andrew Leach, Longman Publications.
2. Computational Chemistry, Guy H. Grant & W. Graham Richards, Oxford University press
3. Computational Chemistry: Introduction to the theory and Applications of Molecular and Quantum Mechanics, Errol Lewars, Springer Publications.
4. Recent advances in Bioinformatics by I. A. Khan and A Khanum
5. Molecular modelling – Basic Principles and Applications by Hans Dieter Holtje and Gerd Folkers, VCH, 1996
6. Introduction to Computational Chemistry by Jensen, Wiley Publishers
7. Bioinformatics – A Primer by P. Narayanan, New Age International, 2005.
8. Introduction to Bioinformatics by Arthur M. Lesk, Oxford University Press (Indian edition), 2002.
9. Principles of Medicinal Chemistry Vol. II by Dr. SS Kadam
10. Bioinformatics by Rastogi
11 . Pharmacy Practice Vol.I and II by Remington

Practicals : Semester- IV

CH (P) 451P: Paper-V (Chemical Kinetics)

- Study of acetone-iodine reaction by spectrophotometry
  - Order w.r.t.[iodine]
  - Order w.r.t. [acetone]
  - Order w.r.t. $[H^+]$
- Study of saponification of ethyl acetate by conductometry:
  - Overall order of the reaction
  - Order w.r.t. [ethyl acetate]
  - Order w.r.t. [NaOH]
- Study of solvolysis of t-butylchloride by conductometry: effect of solvent dielectric constant/ polarizability (methanol/water mixture) on the rate of solvolysis
- Study of oxidation of primary alcohols by dichromate by spectrophotometry: application of Taft equation

CH (P) 452P: Paper-VI (Instrumentation)

Spectrophotometry:

- Estimation of Cu(II) using EDTA
- Estimation of Fe(III) using thiocyanate
- Estimation of Fe(II) using 1,10-phenanthroline
- Estimation of Fe(III) in tap water using thiocyanate by standard addition method
- Simultaneous determination of dichromate and permanganate in a mixture
- Spectrophotmetric titrations:
  - Cu(II) vs EDTA
  - Fe(II) vs 1,10-phenanthroline
- Composition of Cu(II) – EDTA complex by Job's method
- Composition of Fe(II) – phenanthroline complex –
  by Job's method, by mole ratio method, by slope ratio method
- Determination of composition and Gibbs energy of formation of Fe(III) – salicylic acid complex
- Determination of pK_a of methyl red indicator
- Estimation of Mn(II) by spetrophotometry using periodate.

Potentiometry:

- Potentiometric titrations:

  Weak acids vs strong base and calculation of dissociation constants
  Mixture of strong and weak acids vs strong base
  Dibasic acid vs strong base
  Fe(II) vs Ce(IV) and calculation of formal redox potential of Fe(II)/Fe(III)
  Fe(II) vs MnO_4^-
  I^- vs MnO_4^-

Fe(III) vs EDTA
Mixture of halides vs $AgNO_3$
Mixture of KI and KSCN vs $AgNO_3$

Polarography:

- Estimation of Pb^{2+}, Cd^{2+} and Ni^{2+} separately and in a mixture

PHYSICAL -ORGANIC CHEMISTRY SPECIALISATION

SYLLABUS (2012 – 13) ONWARDS

M.Sc. CHEMISTRY(PHYSICAL-ORGANIC CHEMISTRY)

III & IV SEMESTERS

FOR STUDENTS ADMITTED IN THE YEAR (2011 – 12)

REVISED AS PER NEW (CB) SYLLABUS

M.Sc. PHYSICAL ORGANIC CHEMISTRY SPECIALIZATION

Syllabus for III and IV Semesters

(For the batch admitted during the academic year 2011-2012 under the CBCS pattern)

[Under Restructured CBCS Scheme]

(Approved in the P.G. BOS meeting held on 15-9-2012)

Semester - III

	Instruction Hrs/week	Internal assessment marks	Semester exam marks	Total marks	Credits
CH(PO) 301T	4	20	80	100	4
CH(PO) 302T	4	20	80	100	4
CH(PO) 303T	4	20	80	100	4
CH(PO) 304T	4	20	80	100	4
SEMINAR	2			25	1
CH(PO) 351P	9	_	100	100	4
CH(PO) 352P	9	_	100	100	4
Total				**625**	**25**

*Theory: 3 hours ; Practical's: 6 hours

Semester - IV

	Instruction Hrs/week	Internal assessment marks	Semester exam marks	Total marks	Credits
CH(PO) 401T	4	20	80	100	4
CH(PO) 402T	4	20	80	100	4
CH(PO) 403T	4	20	80	100	4
CH(PO) 404T (CB)	4	20	80	100	4
SEMINAR	2			25	1
CH(PO) 451P	9	_	100	100	4
CH(PO) 452P	9	_	100	100	4
Total				**625**	**25**

(**Choice based paper (CB) =** Paper offered by the same Department or other Department in the Science faculty)

*Theory: 3 hours; Practical's: 6 hours

Grand total (all 4 semesters) 2500 marks and 100 credits

M.Sc. PHYSICAL ORGANIC CHEMISTRY SPECIALIZATION
Syllabus for III Semester
(For the batch admitted during the academic year 2011-2012 under the CBCS pattern)
[Under Restructured CBCS Scheme]
(Approved in the P.G. BOS meeting held on 15-9-2012)

CH(PO) 301T: Chemical kinetics, Catalysis and Electrochemistry

PO- 01: Chemical Kinetics-II
PO- 02: Heterogeneous, Phase-transfer& Enzyme catalysis
PO- 03: Polymerization & Kinetics of polymerization
PO- 04: Electrochemistry-II

CH(PO) 302T:Thermodynamics, Supramolecular Chemistry and Nanoparticles

PO- 05:Statistical Thermodynamics
PO- 06: Non equilibrium Thermodynamics
PO- 07: Supramolecular Chemistry
PO- 08: Nanoparticles

CH(PO)303T: Conformational Analysis, Asymmetric synthesis and Synthetic strategies

PO- 09: Conformational Analysis (Cyclic Systems)
PO- 10: Principles of Asymmetric synthesis
PO- 11: Methodology of asymmetric synthesis
PO- 12: Synthetic strategies

CH(PO) 304T: Modern Organic Synthesis

PO- 13: Synthetic Reagents I
PO- 14: Synthetic Reagents II
PO- 15: New synthetic reactions
PO- 16: New techniques and concepts in organic synthesis

CH(PO) 351P: Chemical Kinetics (Paper-V)

CH(PO) 352P:Organic Synthesis and chromatography(Paper-VI)

M.Sc. PHYSICAL ORGANIC CHEMISTRY SPECIALIZATION
III SEMESTER SYLLABUS
(For the batch admitted during the academic year 2011-2012 under the CBCS pattern)
[Under Restructured CBCS Scheme]

Paper I
CH(PO) 301T Chemical kinetics, catalysis and Electrochemistry

PO- 01: Chemical Kinetics-II
PO- 02: Heterogeneous, Phase-transfer& Enzyme catalysis
PO- 03: Polymerization & Kinetics of polymerization
PO- 04: Electrochemistry-II

PO- 01: Chemical kinetics – II (15 hrs)

Review of the transition-state theory. Application to reaction between atoms and molecules. Limitations of the transition-state theory.
Unimolecular reactions: Modification of Lindemann's theory. Hinshelwood treatment, RRK treatment and RRKM treatment.
Reactions in solution: Factors affecting reaction rates in solution. Diffusion-controlled reactions. Influence of dielectric constant and ionic strength on ion-ion, ion-dipole and dipole-dipole reactions. Primary and secondary salt effects.
Kinetic isotope effects: Primary and secondary isotope effects. Solvent isotope effects.
Electron transfer reactions: Inner sphere and outer sphere redox reactions. Marcus theory, the physical model. Marcus cross relation and calculation of rate constant of a bimolecular reaction. Decomposition of N_2O_5. Hydrogen-oxygen reaction and the explosion limits. Decomposition of ethane and acetaldehyde – the Rice-Herzfeld mechanisms.
Fast reactions: Flow methods and the stopped-flow technique. Relaxation methods (T-jump and P-jump). Kinetic equations for chemical relaxation.

PO- 02: Heterogeneous, Phase-transfer and Enzyme catalysis (15 hrs)

Heterogeneous catalysis: Broad categories of catalysts – metals, semiconductors, insulators, zeolites. Steps in heterogeneous catalyzed reactions. Diffusion and adsorption. Mechanism of surface-catalyzed reactions. The Langmuir-Hinshelwood and the Eley-Rideal mechanism. Rate constants and activation energies of surface reactions. Catalytic activity – the determining factors. Cracking and reforming, auto exhaust emissions-catalytic converters

Phase-transfer catalysis (PTC): Principles of phase-transfer catalysis. PTC classification. Role of water in phase-transfer catalyzed reactions. Factors influencing the rate of PTC reactions. Inverse phase transfer catalysis. Mechanism of nucleophilic displacement reactions.

Enzyme kinetics: Enzyme-substrate complex. Specificity of enzyme-catalyzed reactions. Discussion of the various types of forces involved in the formation of E-S complex.

Michaelis-Menten mechanism of enzyme catalyzed reactions involving one and two intermediates. Steady-sate approximation. Derivation of kinetic equations. Evaluation of kinetic parameters. Enzyme irreversible and reversible inhibition. Discussion of equations involved. pH dependence of enzyme-catalyzed reactions.

PO- 03:Polymerization and Kinetics of polymerization (15 hrs)

Classification of polymers. Types of polymerization. Kinetics and mechanism of free radical polymerization. Degree of polymerization, kinetic chain length and chain transfer coefficient – Effect of pressure and temperature on chain polymerization. Kinetics and mechanism of cationic, anionic polymerization. Coordination polymerization and linear stepwise polymerization. Copolymerization reactions and copolymer composition. Reactivity ratios and their determination. Block and graft copolymers.

Polymerization in homogeneous and heterogeneous systems. Bulk, solution, suspension and emulsion polymerizations. Micelle formation and critical micellar concentration. Structure of micelles – spherical and laminar. Reactions assisted by micelle formation. Examples of micelle-catalyzed reactions and their mechanisms

PO- 04: Electrochemistry – II (15 hrs)

The electrode-electrolyte interface. The electrical double layer. The Helmholtz-Perrin parallel-plate model, the Gouy-Chapman diffuse-charge model and the Stern model. Quantum aspects of charge transfer at the interfaces. Tunneling.

Electrodics. Charge transfer reactions at the electrode-electrolyte interface. Exchange current density and overpotential. Derivation of Butler-Volmer equation. High field approximation. Tafel equation - low field - equilibrium, Nernst equation. The symmetry factor and its significance.

Corrosion: Electrochemical corrosion. Short-circuited energy producing cell. Homogeneous theory of corrosion. The corrosion current and the corrosion potential. Potential-pH (Pourbaix) diagrams of iron. Protection against corrosion. Corrosion inhibitors. Corrosion inhibition by organic molecules.

Electro-organic synthesis. Reduction of carboxylic acids and nitro compounds, the elctrodimerization of acrylonitrile to adiponitrile.

Batteries. Battery parameters. Energy density and power density. Measures of battery performance. Primary and secondary batteries Zn/MnO_2, lead-acid and Ni-Cd batteries and lithium batteries.

Fuel cells. H_2/O_2 and methanol/O_2 fuel cells. Use of porous electrodes in fuel cells. Advantages and limitations of fuel cells. Photovoltaic cells. Semiconductor based photoelctrochemical cells.

Books suggested:

1. Chemical Kinetics, K. J. Laidler, McGraw Hill, New York.
2, Kinetics and Mechanism, A. A. Frost & R. G. Pearson, John Wiley & sons.
3. Kinetics and Mechanism of Chemical Transformations, J. Rajaraman & J.Kuriacose. McMillan.
4. Chemical Kinetics and Reaction Mechanisms, J. H. Espenson, McGraw Hill.
5. Physical Organic Chemistry, N. S. Isaacs, ELBS.
6. The Physical basis of Organic Chemistry, Howard Maskill, Oxford University Press.
7. Rates and Equilibriums of Organic Reactions, J. E. Leffler & E. Grunwald, Dover publications.
8. Reaction Dynamics, edited by N. Sathyamurthy, Narosa Publishing House.
9. Physical Chemistry of Surfaces, A. W. Adamson & A. P. Gast, Wiley.
10. Physical Chemistry, Ira N. Levine, McGraw Hill.
11. Atkin's Physical Chemistry, P. Atkins & Julio de Paula, Oxford University Press.
12. The New Chemistry, Editor-in-chief Nina Hall, Cambridge University Press.
13. Micelles- Theoretical and Applied aspects, V. Moroi, Plenum.
14. Physical Chemistry: A molecular approach, McQuarie Simon, Viva Books Pvt. Ltd. New Delhi.
15. Textbook of Polymer Science, F. W. Billmeyer Jr, John Wiley & sons.
16. Polymer Science, V. R. Gowarikar, N. V. Viswanathan & J. Sreedhar, Wiley Eastern.
17. Contemporary Polymer Chemistry, H. R. Alcock & F. W. Lambe, Prentice Hall.
18. Physics and Chemistry of Polymers, J. M. G. Cowie, Blackie Academic and Professional.
19. Polymer Chemistry, B. Vollmert.
20. Physical Chemistry of Polymers, A. Tagers, Mir Publishers.
21. A Guide to Lasers in Chemistry, G. R. Van Hecke & K. K. Karukstis, Jones and Bartlett Publishers.
22. Lasers in Chemical and Biological Sciences, S. Chopra & H. M. Chawla, Wiley Eastern Ltd.
23. Modern Electrochemistry, J. O. M. Bockris & A. K. N. Reddy, Plenum.
24. Introduction to Electrochemistry, S. Glasstone.
25. Fundamental Principles of Modern Electroplating, Lowenheim, John Wiley.
26. Industrial Electrochemistry, D. Pletcher, Chapman & Hall.

Paper-II
CH(PO) 302T: Thermodynamics, Supramolecular Chemistry & Nanoparticles

PO- 05: Statistical Thermodynamics
PO- 06: Non equilibrium Thermodynamics
PO- 07: Supramolecular Chemistry
PO- 08: Nanoparticles

PO- 05: Statistical Thermodynamics: (15 hrs)

Concepts of distribution and probability. Estimation of probability and the most probable distribution. Systems composed of noninteracting particles. Derivation of Boltzmann distribution law.

The molecular partition function. Systems composed of interacting particles. The concept of ensemble and canonical ensemble. Canonical partition function and its relation to molecular partition function. The factorization of molecular partition function – translational, rotational, vibrational and electronic partition functions. Derivation of expressions for translational, rotational (diatomic) and vibrational partition functions. The relationship between partition functions and thermodynamic functions. Law of equipartition energy.

Specific heats of solids – Einstein equation of heat capacity of solids – derivation. Explanation of heat capacity at very low and very high temperatures – Dulong and Petits Law. Debye theory.

The entropy of a monoatomic ideal gas. The Sackur-Tetrode equation- derivation. Mean translational and vibrational energies.

The relation between equilibrium constant and partition function- derivation.
Basic ideas of Bose-Einstein statistics and Fermi-Dirac statistics and comparison of these with Maxwell-Boltzmann statistics.

PO- 06 : Non-equilibrium Thermodynamics (15 hrs)

Thermodynamic criteria for non-equilibrium states. Entropy production in irreversible processes. Entropy production in heat flow and entropy production in material flow.
Fluxes and forces. Linear flux-force relations. Phenomenological equations and coefficients. Microscopic reversibility. Onsager reciprocal relations. Application of Onsager relations to electrokinetic phenomena – electro osmotic pressure and streaming current. The Onsager relations and the principle of detailed balance.

Liquid junction potentials – derivation of equation for liquid junction potential in terms of transport numbers using Onsager relations. Steady states. Principle of minimum entropy production. Irreversible thermodynamics as applied to biological systems – examples viz.,

sodium potassium pump, glucose transport. Application to thermoelectric circuits. Seebeck and Peltier effect.

PO- 07: Supramolecular Chemistry (15 hrs)

Molecules, super molecules and supramolecules.Molecular recognition – factors involved. Ionophores. Molecular receptors – design principles. Molecular receptors for alkali metal ions, ammonium ions, anions and neutral molecules.

Types of interactions between host and guest molecules. Thermodynamics of host-guest complexation. Enthalpy and entropy contributions. Complexation free energies.

Crown ethers, cryptands, spherands, cyclodextrins and calixaranes.
Threading of a linear molecule through a cyclic molecule. Creation of rotaxanes and catenanes.

Applications. Supramolecular catalysis- examples. Transport of ions across membranes. Molecular wires and molecular switches.

PO- 08: Nanoparticles and their applications (15 hrs)

Introduction to nano particles. Preparation of nano particles –various methods- RF plasma, chemical methods, thermolysis, pulsed laser methods, optical and electrical properties of nanoparticles. Characterization of nano particles-experimental methods-powder X-ray diffraction, transmission electron microscopy (TEM), scanning electron microscopy (SEM) and atomic force microscopy(AFM).

Reduced dimensionality in solids – zero dimensional systems, fullerenes, quantum dots. Optical properties of quantum dots. One dimensional systems, carbon nano tubes, electric, mechanical and other properties.

Applications of nano particles in – photocatalysis, laser and light emitting diodes, optical filters, optical band gap materials. Use of carbon nano tubes in fuel cells and catalysis.

Books suggested:

1. Elements of Statistical Thermodynamics, L. K. Nash, Addison – Wesley.
2. Introduction to Statistical Thermodynamics, T. L. Hill, Addison – Wesley.
3. Statistical Thermodynamics, M. C. Gupta, New Age International.
4. Atkin's Physical Chemistry, P. Atkins & Julio de Paula, Oxford University Press.
5. Molecular Thermodynamics, D. A. McQuarrie & J. D. Simon, University Science Books.
6. Text book of Biochemistry by L Stryer, W H. Freeman & Company.
7. Biophysical Chemistry, Cantor & Schimmel, W. H. Freeman & Company.
8. Principles of Physical Biochemistry, Kensal E vanHolde, W. Curtis Johnson & P Shing Ho, Prentice Hall.

9. Physical Biochemistry: Principles and applications, David Sheehan, John Wiley.
10. Advanced physical chemistry by Gurtu and Gurtu.
11. Physical chemistry by Puri and Sharma.
12. Materials Science & Engineering – A First Course, V. Raghavan, Prentice Hall.
13. Introduction to Nanotechnology, C. P. Poole Jr. & F. J. Owens, John Wiley & Sons.
14. Nanostructured Materials and Nanotechnology, edited by Hari Singh Nalwa, Academic Press.
15. Self Assembled Nanostructures, Jin Zhang, Zhong-lin Wang, Jun Liu, Shaowei Chen & Gang-Yu-Liu, Kluwer Academic/Plenum.
16. Introduction to theoretical Organic Chemistry and molecular modeling by W.B.Smith, VCH,Weinhein.
17. Physical Organic chemistry, N. S.Isaaçs.
18. Suprarnolecular Chemistry - concepts and perspectives by J M .Lehn.
19. Supramolecular Chemistry – Fundamentals and Applications Advanced Textbook Katsuhiko Ariga · Toyoki Kunitake.(e- Book).
20. The New Chemistry, Editor-in-chief Nina Hall, Cambridge University Press.
21. Principles and methods in Supramolecular Chemistry, Hans-Jorg, Schneider & . Ytsimirsky, John Wiley & Sons.
22. Analytical Chemistry of Macrocyclic and Supramolecular Compounds, S. M. Khopkar, Narosa Publishing House.

Paper III
CH (PO) 303T: Conformational Analysis, Asymmetric Synthesis and Synthetic Strategies

PO- 09: Conformational Analysis (Cyclic Systems)
PO- 10: Principles of Asymmetric synthesis
PO- 11: Methodology of asymmetric synthesis
PO- 12: Synthetic Strategies

PO- 09: Conformational analysis (Cyclic systems) (15 hrs)

Study of conformations of cyclohexane, mono, di and polysubstituted cyclohexanes, cyclohexene, cyclohexanone (2-alkyl and 3 -alkyl ketone effect), 2-halocyclohexanones, cyclopentane, cyclobutane, cycloheptane and cyclooctane. Stereo chemistry of bicyclo[3,3,0]octanes, hydrindanes, decalins and perhydroanthracenes.

Conformational structures of piperidine, N-Methylpiperidine, tropane, tropine, pseudotropine, decahydroquinoline and quinolizidine. Conformational effects on the stability and reactivity of diastereomers in cyclic molecules - steric and stereo electronic factors – examples. Factors governing the reactivity of axial and equatorial substituents in cyclohexanes. Stereochemistry of addition to the carbonyl group of a rigid cyclohexanone ring.

PO- 10: Principles of asymmetric synthesis (15 hrs)

Introduction and terminology: Topocity in molecules Homotopic, stereoheterotopic (enantiotopic and diastereotopic) groups and faces- symmetry, substitution and addition criteria. Prochirality nomenclature: Pro-R, Pro-S, Re and Si.

Stereoselective reactions: Substrate stereoselectivity, product stereoselectivity, enantioselectivity and diastereoselectivity. Conditions for stereoselectivity: Symmetry and transition state criteria, kinetic and thermodynamic control. Methods for inducing enantio and diastereoselectivity.

Analytical methods: % Enantiomeric excess, enantiomeric ratio, optical purity, % diastereomeric excess and diastereomeric ratio. Techniques for determination of enantioselectivity: Specific rotation, Chiral ^{1}H nmr, Chiral lanthanide shift reagents and ChiralHPLC.

PO- 11: Methodology of Asymmetric Synthesis (15 hrs)

Strategies in Asymmetric Synthesis:

l. Chiral substrate controlled 2. Chiral auxiliary controlled 3.Chiral reagent controlled and 4.Chiral catalyst controlled.

1. Substrate controlled asymmetric synthesis: Nucleophilic additions to chiral carbonyl compounds. 1,2- asymmetric induction, Cram's rule and Felkin-Anh model.

2. Chiral auxiliary controlled asymmetric synthesis: α-Alkylation of chiral enolates, azaenolates, imines and hydrazones. 1, 4-Asymmetric induction and Prelog's rule. Use of chiral auxiliaries in Diels-Alder reaction.

3. Chiral reagent controlled asymmetric synthesis: Asymmetric reductions using BINAL-H. Asymmetric hydroboration using IPC_2 BH and $IPCBH_2$.

4. Chiral catalyst controlled asymmetric synthesis: Sharpless and Jacobsen asymmetric epoxidations. Sharpless asymmetric dihydroxylation. Asymmetric hydrogenations using chiral Wilkinson biphosphine and Noyori catalys. Enzyme mediated enantioselective synthesis.

5. Asymmetric aldol reaction, Diastereoselective aldol reaction (chiral enolate & achiral aldehydes and achiral enolate & chiral aldehydes) its explanation by Zimmerman-Traxel model.

PO- 12: Synthetic Strategies (15 Hrs.)

Synthetic Strategies : Terminology: target, synthon, synthetic equivalent, functional group interconversion (FGI), functional group addition, functional group elimination. Crieteria for selection of target. Linear and convergent synthesis. Retrosynthetic analysis and synthesis involving chemoselectivity, regioselectivity, reversal of polarity and cyclizations. Strategic bond: Crieteria for disconnection of strategic bonds. Importance of the order of events in organic synthesis. One group and two group C-X disconnections. One group C-C disconnections. Alcohol and carbonyl compounds. Two group C-C disconnections; Diels-Alder reaction, 1,3-difunctionalised compounds, 1,5-difunctionalised compounds, Michael addition and Robinson annulation, synthesis of (+)disparlure by retrosynthetic approach.

Recommended Books:

1. Stereochemistry of organic compounds — Principles & Applications D Nasipuri
2. Stereochemistry of Carbon compounds by Ernest L Eliel & Samuel H. wilen

3. Stereochemistry: Conformation & Mechanism by P S Kalsi
4. The third dimension in organic chemistry, by Alan Bassendale
5. Stereo selectivity in organic synthesis by R S Ward.
6. Asymmetric synthesis by Nogradi
7. Asymmetric organic reactions by it) Morrison and HS Moschcr
8. Principles in Asymmetric synthesis by Robert E. Gawley & JEFFREY AUBE
9. Stereo differentiating reactions by Izumi
10. Some modern methods of organic synthesis by W Carruthers
11. Guidebook to organic synthesis, by R K Meckie, D M Smith & R A Atken
12. Organic synthesis by Michael B Smith
13. Organic synthesis by Robert Ireland.
14. Organic synthesis-The disconnection approach by Stuart Warren.
15. Problems in organic synthesis by Stuart Warren.
16. Organic synthesis by Willis and Willis.

Paper IV– CH (PO) 304T: Modern Organic Synthesis

PO- 13: Synthetic Reagents I
PO- 14: Synthetic Reagents II
PO- 15: New Synthetic reactions
PO- 16: New techniques and concepts in organic synthesis

PO-13: Synthetic Reagents I (15 hrs)

*i) Oxidations***:** a) Alcohol to carbonyls; Cr^{VI} oxidants (Jones reagent, PCC. PDC) IBX, DMP, CAN, TEMPO, TPAP, Swern oxidation b) alkenes to diols: Prevost and Woodward oxidation c). Oxidative cleavage of 1,2-diols: Periodic acid and Lead tetraacetate d). Oxidation of allylic and benzylic C-H bonds: DDQ and SeO_2.

*ii) Reductions***:** a). Catalytic hydrogenation: Homogenous (Wilkinsons's catalytic hydrogenation) and heterogeneous catalytic reduction. b) Non-metallic reductions: Diimide reduction c) Dissolving metal reductions: Birch reduction. d) Nucleophilic metal hydrides: $LiAlH_4$, $NaBH_4$, and their modifications.e) Electrophilic metal hydrides: BH_3, AlH_3 and DIBAL. f) Hydrogenolysis g) use of tri-n-butyl tin hydride.

*iii) Protecting groups***:** a) Protection of alcohols by ether, silyl ether and ester formation b). Protection of 1,2-diols by acetal, ketal and carbonate formation c) Protection of amines by acetylation, benzoylation, benzyloxycarbonyl, t-butyloxycarbonyl, fmoc and triphenyl methyl groups. d) Protection of carbonyls by acetal, ketal and thiol acetal (Umpolung) groups. e) Protection of carboxylic acids by ester and ortho ester (OBO) formation.

PO-14: Synthetic Reagents II (15 hrs)

*i) Organometallic Reagents***:** a) Preparation and application of the following in organic synthesis: 1) Grignard, 2) Organo lithium and 3) Organo copper reagents b) Organo boranes in C-C bond formation c). Organo silicon reagents: reactions involving β-carbocations and α-carbanions, utility of trimethyl silyl halides, cyanides and triflates.

*ii) Carbonyl methylenation***:** a) Phosphorous ylide mediated olefination: 1) Witting reaction, 2) Homer-Wordworth Emmons reaction 3) a) Silyl ylide mediated olefination: Peterson olefination b) Titanium- Carbene mediated olefination: 1) Tebbe reagent, 2) Petasis reagent d) Olefination by Nysted reagent

PO-15: New Synthetic reactions (15 hrs)

*1. Metal mediated C-C and C-X coupling reactions***:** Suziki coupling, Heck reaction, Stille coupling, Sonogishira cross coupling, Buchwald-Hartwig coupling Reaction and Negishi-Kumada.

2. C=C Formation Reactions: Shapiro reaction, Bamford-Stevens reaction, McMurrey reaction, Julia-Lythgoe olefination and Peterson's stereoselective olefination.

3. Multicomponent Reactions: Ugi, Passerini, Biginelli, Hantzsch and Mannich reactions.

4. Ring Formation Reactions: Pausan-Khand reaction, Bergman cyclisation, Nazerov cyclisation.

5. Click Chemistry: Criteria for Click reaction, Sharpless azides cycloadditions.

6.Metathesis: Grubb's 1st and 2nd generation catalyst, Olefin cross coupling metathesis(OCM), ring closing metathesis(RCM), ring opening metathesis(ROM), applications.

7. Other important synthetic reactions: Baylis-Hilman reaction, Eschenmoser-Tanabe fragmentation, Mitsunobu reaction, Stork-enamine reaction and Michael reactions.

PO-16: New techniques and concepts in organic synthesis (15 hrs)

1. Techniques in peptide synthesis: Solid phase peptide synthesis, synthesis of cross linked Merrifield resin, commonly used resins (Rink resin, Wang resin and Ellman resin) and drawbacks of solid phase synthesis.

2. Solid phase oligodeoxynucleotide synthesis: Triester pathway and phosphoramidite pathway .

3. Olegosaccharide synthesis: Protection of hydroxyl groups, cylic oxocarbenium ion, glycosyl donors and glycosiyl acceptors, Kahne glycosidation, convergent and linear oligosaccharide synthesis.

4. Phase Transfer catalysis: Onium and Crown ethers as PTC.

5.Tandem synthesis: Tandem reactions; conjugate addition-aldol reaction, polymerization-cyclisation, electrocylic-Diels Alder reaction.

6. Baldwin Rules: Exo and Endo cyclisation, tetrahedral, trigonal and diagonal systems, favoured and disfavoured cyclisations.

7. Chiron approach in organic synthesis: Nature's chiral pool, carbohydrates, amino acids, hydroxy acids, terpenes as chiral precursors. Synthesis of shikimic acid from D-arabinose, furanonycin from D-glucose, S-(-)-ipsenol from S-leucine. 8) Determination of absolute configuration: Mosher's methods.

Recommended Books:

1. Some modern methods of organic synthesis by W. Carruthers.
2. Guidebook to organic synthesis, by R K Meckie, D M Smith & R A Atken.
3. Organic Synthesis by O House.
4. Organic synthesis by Micheal B Smith.
5. Reagents for organic synthesis, by Fieser & Fieser, Vol 1-11 (1984).
6. Organic synthesis by Robert E Ireland.
7. Organic Synthesis-The disconnection approach by S Warren.

8. Organic Synthesis by C Willis and M Willis.
9. Handbooks of reagents for organic synthesis by Reich and Rigby, Vol-I-IV.
10. Problems on organic synthesis by Stuart Warren.
11. Total synthesis of natural products: the Chiron approach by S. Hanesian.
12. Organic chemistry Claydon and other 2005.

SEMESTER III LABORATORY COURSES

PAPER V (Lab)-CH(PO) 351P: Chemical Kinetics

Data analysis: Significant figures, Precision and accuracy, Mean and standard deviation; absolute and relative errors; linear regression; covariance and correlation coefficient.

1.Study of peroxydisulphate-iodide reactions;

a) Individual orders of the reactants by isolation and initial rate methods
b) Effect of temperature on reaction rate
c) Effect of ionic strength on reaction rate

2.Study of peroxydisulphate-iodide clock reaction; effect of ionic strength on uncatalysed and Cu(II) catalysed reactions.

3.Study of acetone-iodine reaction: by titrimetry/photometry

a).Order w.r.t. iodine b).Order w.r.t. acetone c). Order w.r.t. [H+]

4.Study of saponification of ethyl acetate by conductometry:

a). Overall order of the reaction b). Order w. r. to ethylacetate c).Order w.r. to NaOH

5.Study of solvolysis of t-butylchloride by conductometry: effect of solvent dielectric constant/polarizability (methanol/water mixture) on the rate of solvolysis.

6.Study of oxidation of primary alcohols by dichromate by spectrophotometry: application of Taft equation.

7. Study of polymerization of styrene and effect of initiator concentration on rate of polymerization.

Note: The Data obtained in all the experiments are to be analysed by the students both by the usual graphical methods and by regression (linear/nonlinear) techniques using a PC.

Suggested books:

1. A textbook of pratical organic chemistry by A I Vogel, Vol 1&2.
2. Unitized experiments in organic chemistry by R Q Brewster and others.
3. Handbook of organic analysis by H T C Clarke.
4. Practical Organic Chemistry by Mann and Saunders.

PAPER VI -CH(PO)352P: Chromatography & Synthesis of Organic compounds

1.**Thin layer chromatography**: Determination of purity of a given sample monitoring the progress of chemical reactions and column chromatographic separations , identification of unknown organic compounds by comparing the Rf values of known standards and preparative TLC for separations of mixtures.

2.**Separation/Purification by column chromatography**: Separation of a mixture of ortho and para-nitroanilines using silicagel as adsorbant and chloroform as the eluent. The column chromatography should be monitored by TLC. Purification of commercial sample of anthracene by column chromatography (using silica gel as adsorbant and n-hexane as eluent).

3. **Laboratory synthesis of the following compounds**: 2-Phenyl indole (Fischer- Indole synthesis), 2,5-Dihydroxy acetophenone (Fries reaction), 7-hydroxy coumarin (Pechmann synthesis), Photo-dimerization of maleic anhydride, Benzanilide (Beckmann rearrangement), Benzilic acid from benzoin (rearrangement), Vanillyl alchohol from vanillin ($NaBH_4$ reduction), 4-Nitoacetanilide from acetanilide , Benzimidazoles and Benzimidazolines by reaction of o-phenylenediamine with aromatic aldehydes and carboxylic acids.

Suggested books:

1.A textbook of pracical organic chemistry by A I Vogel, Vol 1&2.

2.Unitized experiments in organic chemistry by R Q Brewster and others.

3.Handbook of organic analysis by H T C Clarke.

4.Practical Organic Chemistry by Mann and Saunders.

M.Sc. PHYSICAL ORGANIC CHEMISTRY SPECIALIZATION
IV SEMESTER SYLLABUS
(For the batch admitted during the academic year 2011-2012 under the CBCS pattern)
[Under Restructured CBCS Scheme]

CH(PO) 401T: Spectroscopy , photochemistry and lasers in chemistry

PO- 17 : Physical principles of spectroscopy & Vibrational spectroscopy
PO- 18 : X-Ray Spectroscopy & Diffraction techniques
PO- 19: Photochemistry – II
PO- 20: Lasers in chemistry

CH(PO) 402T: Quantum Chemistry and Group Theory

PO- 21: Applications of Schrödinger equation
PO- 22: Angular momentum & approximate methods
PO- 23: Bonding in molecules
PO- 24: Group Theory

CH (PO) 403T: Organic Spectroscopy and Pericyclic reactions.

PO-25: ^{13}C NMR spectroscopy
PO-26: 2D NMR techniques and ORD
PO-27: Pericyclic reactions I
PO-28: Pericyclic reactions II

Paper-IV CH (PO) 404T(CB_1): Heterocyclics , Biomolecules, Green chemistry and Principles of drug design and discovery

PO-(CB1)- 29: Five and six membered heterocyclics with two hetero atoms
PO-(CB1)- 30: Biomolecules
PO-(CB1) - 31: Green chemistry
PO-(CB1) - 32: Principles of drug design and discovery

CH (PO) 404T(CB_2): Modern material Chemistry & Combinatorial Chemistry

PO-(CB2)-29: Types of materials, Conducting Organics and NLO materials
PO-(CB2)-30: Functional Polymers
PO-(CB2)-31: Dynamics of biopolymers
PO-(CB2)-32: Combinatorial Chemistry

CH (PO) 404T(CB_3): Biopolymer chemistry

PO-(CB3)- 29: Bioenergetics & physical properties of biopolymers
PO-(CB3)-30: Biological membranes & binding of ligands by biopolymers
PO-(CB3) -31: DNA, genes & cloning
PO-(CB3) -32: Bioinformatics

Paper (Lab)-CH(PO) 451P: Instrumentation (paper-VII)

Paper (Lab) CH(PO) 452P : Separation and identification of organic compounds and spectral analysis (paper-VIII)

M.Sc. PHYSICAL ORGANIC CHEMISTRY SPECIALIZATION
IV SEMESTER SYLLABUS
(For the batch admitted during the academic year 2011-2012 under the CBCS pattern)
[Under Restructured CBCS Scheme]

Paper-I

CH(PO) 401T: Spectroscopy , photochemistry and lasers in chemistry

PO- 17 : Physical principles of spectroscopy & Vibrational spectroscopy
PO- 18 : X-Ray Spectroscopy & Diffraction techniques
PO- 19: Photochemistry – II
PO- 20: Lasers in chemistry

PO-17: Physical principles of spectroscopy & Vibrational spectroscopy (15 Hrs)

Interaction of electromagnetic radiation with matter. Absorption and emission of radiation. Induced absorption, spontaneous emission and stimulated emission. Einstein coefficients. Selection rules. Oscillator strength. Line width and natural line broadening. Doppler broadening. Intensity of spectral lines.

Infrared spectroscopy: Anharmonic oscillator.Morse potential energy diagram.Vibration – rotation spectroscopy, P, Q, R branches. Vibration – rotation spectra of polyatomic molecules – linear, symmetric top and asymmetric top molecules. Principles of FTIR.

Raman spectroscopy: Classical and quantum theories of Raman effect. Pure rotational, vibrational and vibrational – rotational Raman spectra. Selection rules. Depolarization factors of Raman lines and their relevance. Instrumentation. Typical applications of Raman spectroscopy. Principles of Resonance Raman spectroscopy. Principles of coherent antiStokes Raman spectroscopy (CARS)

PO-18: X-ray Spectroscopic Techniques & Diffraction techniques (15 Hrs)

X-Ray fluorescence(XRF) spectra : Absorption technique, Absorption Edge Fine Structure(AEFS) spectra and Extended X-Ray Absorption Fine Structure(EXAFS) spectra.

X-ray diffraction: Bragg condition. Miller indices. Experimental methods of X-ray diffraction. Laue method and Debye-Scherrer method. Primitive and nonprimitive unit cells. Index reflections. Identification of unit cells from systematic absences in diffraction

pattern. Structure factor and its relation to intensity and electron density. Description of the procedure for an X-ray structure analysis. Typical examples.

Electron diffraction. Scattering intensity versus scattering angle. Wierl equation. Measurement technique. Elucidation of structure of simple gas phase molecules.

PO- 19: Photochemistry – II **(15 Hrs)**

Formation of excimers and exciplexes – PE diagram and quantum yields. Energy transfer mechanism for bimolecular quenching. Long-range coulombic energy transfer – critical transfer distance. Short-range electron exchange energy transfer. Triplet-triplet energy transfer and sensitization. Experimental study of radiative transitions. Emission spectroscopy. Emission quenching measurements. Flash photolysis.

Organic photochemistry. Properties of (n, π^*) and (π, π^*) states.
Photochemistry of alkenes. Cis-trans isomerisation, di-π- methane rearrangement.
Photochemistry of carbonyl compounds. Norrish type-I reactions. Photoreduction. Norrish type-II reactions. Addition of carbonyl to carbon-carbon multiple bonds (Paterno-Buchi) reaction. Barton reaction. Singlet oxygen – photooxidation and reactions with C=C compounds.

Electronic transitions in transition metal complexes. Ligand field (LF) and charge transfer (CT) electronic states. $Ru(bpy)_3^{2+}$ as sensitizer for photoredox reactions, examples. Photochemical cleavage of water.

PO- 20: Lasers in Chemistry **(15 Hrs)**

General principles of laser action. Stimulated emission. Rates of absorption and emission. Einstein coefficients. Population inversion. Three-level and four-level laser systems. Pumping. Laser cavity – resonant modes. Characteristics of laser light. Laser pulses and their characteristics. Pulse production, Q-switching. Pulse modification, mode-locking. Practical lasers. Solid-state lasers, gas lasers, chemical and excimer lasers. Examples.

Applications of lasers in chemistry. Femtochemistry. The pump-probe technique. Time-resolved spectroscopy. Photodissociation of ICN. Formation and dissociation of CO-hemoglobin complex. Conversion of ethylene to cyclobutane. Bond selectivity in chemical reactions – the reaction between hydrogen atoms and vibrationally excited HDO molecules.

Lasers and multiphoton spectroscopy – underlying principles. Two-photon spectra of diphenyloctatetraene. Lasers in fluorescence spectroscopy and Raman spectroscopy.

Books suggested:

1. Modern Spectroscopy, J. M. Hollas, John Wiley & sons
2. Fundamentals of Molecular Spectroscopy, Banwell & McCash
3. Introduction to Molecular Spectroscopy, G. M. Barrow, McGraw Hill
4. Molecular Spectroscopy, J. D. Graybeal, McGraw Hill
5. Basic principles of Spectroscopy, R. Chang, McGraw Hill
6. Physical Methods in Chemistry, R. S. Drago, W.B. Saunders Co., 1977.
7. Physical Methods for Chemists, Russell S. Drago Second edition, Saunders College Publishing, 1992.
8. Vibrational Spectroscopy: Theory and Applications, D. N. Sathyanarayana, New Age International
9. Introduction to Raman Spectroscopy, J. R. Ferraro & K. Nakamoto, Academic Press
10. X-ray diffraction procedures for polycrysralline and amorphous materials, H. P. Klug & L. E. Alexander, John Wiley
11. Solid state chemistry and its application, A. R. West.
12. Molecular Photochemistry, N. J. Turro, W. A. Benzamin
13. Fundamentals of Photochemistry, Rohatgi-Mukherjee, Wiley Eastern Ltd.
14. Essentials of Molecular Photochemistry, A. Gilbert & J. Baggott, Blackwell Science
15. Introduction to Molecular Photochemistry, C. H. J. Wells, Chapman and Hall
16. Inorganic Photochemistry, J.Chem. Educ. vol. 60 No. 10, 1983.
17. Atkin's Physical Chemistry, P. Atkins & Julio de Paula, Oxford University Press.
18. A. Guide to Lasers in Chemistry G. R. Van Heck and K.K. karukstis, Jones & Bartlett Publishers.
19. Lasers in Chemical & Biological Sciences S. Chopra & H. M. Chawla Wiley Eastern Ltd.

Paper II

CH(PO) 402T: Quantum Chemistry and Group Theory

PO- 21: Applications of Schrödinger equation
PO- 22: Angular momentum & approximate methods
PO- 23: Bonding in molecules
PO- 24: Group Theory

PO- 21: Applications of Schrödinger equation (15 Hrs)

Systems with discontinuity in the potential field. A simple potential barrier. A potential barrier with a finite thickness. Quantum mechanical tunneling – examples - α-particle emission, inversion of NH_3, hydrogen transfer reactions.

The harmonic oscillator – detailed treatment. Wave functions and energies. Vibration of a diatomic molecule – harmonic oscillator model.

The rigid rotator – detailed treatment. Wave functions and energies. Spherical harmonics. Rigid rotator as model for a rotating diatomic molecule.

The hydrogen atom – detailed treatment. Angular and radial functions. Atomic orbitals. Measurability of the ground-state energy of hydrogen atom. Orthonormal nature of hydrogen-like wave functions. Probability calculations.

Atoms in external field, Zeeman and anomalous Zeeman effect.

PO- 22: Angular momentum & approximate methods (15 Hrs)

Angular momentum operators. Commutation relations of angular momentum operators and their consequence. Eigen functions of L^2 and Lz and the eigen values. Magnitude and orientation of angular momentum vectors.

Electron spin. Spin operators. Pauli principle and the Pauli exclusion principle. Atomic and molecular term symbols.

Approximate methods. The variation method. Constuction of variation function by the method of linear combinations. Secular equations and secular determinant. H and He atom.

Born-Oppenheimer approximation.MO theory of H_2^+ ion. Calculation of MO's and their energies. Evaluation of the overlap integral. Probability curves and energy diagram.MO theory of H_2 molecule. Calculation of energy.

Perturbation theory for non-degenerate states. Application of perturbation theory to particle in a one dimensional box moving with a steadily varying potential energy.First order correction to the energy and the wave function.

PO- 23: Bonding in molecules **(15 Hrs)**

MO theory of polyatomic molecules (general ideas). MO treatment of H_2O. Symmetry-adapted linear combinations ex: MO's of H_2O.Concept of hybridization – sp, sp^2, and sp^3 hybrid orbitals.

Semi empirical MO methods.
The Huckel theory of conjugated systems. HMO calculations on ethylene, allyl system, butadiene, cyclopropenyl system and benzene. π–electron charges and bond orders and free valence values. Aromaticity and 4n+2 rule.

The use of molecular symmetry for simplification of secular determinants of cyclopropenyl system, cyclobutadiene and benzene. Extension of the Huckle's approach to molecules containing heteroatoms. Inclusion of overlap integrals. Treatment of hybrid and unusually oriented orbital. Simple Mnemonic device for obtaining MO energies. electrocyclic reactions, cycloaddition reactions.

PO- 24: Group Theory **(15 Hrs)**

Matrices: Addition and multiplication of matrices. Diagonal matrix. Unit matrix. Transpose of a matrix. Adjoint of a matrix. Inverse of a matrix. The determinant of a square matrix. Expansion of a determinant. Properties of determinants.

Symmetry operations forming a group. Classes of symmetry operations. Matrix representation of symmetry operations and point groups. Generation of representations for point groups. Reducible and irreducible representations.

The Great Orthogonality theorem (proof not required) and its consequences. Relation between reducible and irreducible representations. Character tables. Construction of character tables for C_{2V} and C_{3V} groups.

Quantum mechanics and group theory. Wave functions as bases for irreducible representations. The direct product – vanishing of integrals. Projection operators. Symmetries of vibrations. IR and Raman activity.

Books suggested:

1. Quantum Chemistry, Ira N. Levine, Prentice Hall.
2. Introduction to Quantum Chemistry, A. K. Chandra, Tata McGraw Hill.
3. Elementary Quantum Chemistry, F. L. Pilar, McGraw Hill.

4. Molecular Quantum Mechanics, P. W. Atkins & R. S. Friedman, Oxford University Press.
5. Coulson's Valence, R. McWeeny, ELBS.
6. The Chemical Bond, J. N. Murrel, S. F. A. Kettle & J. M. Tedder, John Wiley.
7. Elements of Statistical Thermodynamics, L. K. Nash, Addison – Wesley.
8. Introduction to Statistical Thermodynamics, T. L. Hill, Addison Wiley.
9. Statistical Thermodynamics, M. C. Gupta, New Age International.
10. Symmetry and Spectroscopy of Molecules, K. Veera Reddy, Second Edition, New Age International (P) Limited Publishers (2009).
11. Chemical Applications of Group Theory, F. A. Cotton, 3rd edition, Wiley NY (1990)
12. Symmetry and Group Theory In Chemistry, Mark Ladd, Harwood Publishers, London (2000).
13. Symmetry Through the Eyes of a Chemist, I. Hargittai and M. Hargittai, 2nd Edition, Plenum Press, NY (1995).
14. Molecular Symmetry and Group Theory, Robert L. Carter, John Wiley & Sons (1998).
15. Group Theory for Chemists, G. Davidson, Macmillan Physical Science Series (1991).
16. Molecular Symmetry, Schoenland.

Paper III

CH (PO) 403T: Organic Spectroscopy and Pericyclic reactions.

PO-25: ^{13}C NMR spectroscopy
PO-26: 2D NMR techniques and ORD
PO-27: Pericyclic reactions I
PO-28: Pericyclic reactions II

PO-25: ^{13}C NMR spectroscopy (15 Hrs)

CW and PFT techniques. Types of ^{13}C nmr spectra: undecoupled, proton- decoupled and off-resonance decoupled (ORD) spectra. ^{13}C chemical shifts, factors affecting the chemical shifts, chemical shifts of organic compounds. Calculation of chemical shifts of alkanes, alkenes and alkynes. Homonuclear (^{13}C,^{13}C J) and heteronuclear (^{13}C,^{1}H J and ^{13}C- ^{2}H J) coupling. Applications of ^{13}C-NMR spectroscopy: Structure determination, stereochemistry, reaction mechanisms and dynamic processes in organic molecules. ^{13}C-NMR spectral editing techniques: Principle and applications of APT, INEPT and DEPT methods.

PO-26: 2D NMR techniques and ORD (15 Hrs)

1. 2D-NMR techniques: Principles of 2D NMR, Classification of 2D-experiments. 2D-J-resolved spectroscopy. Homonuclear and Heteronuclear 2D-J-resolved spectroscopy. Correlation spectroscopy (COSY) HOMO COSY (^{1}H-^{1}H COSY) , TOCSY (Total Correlation Spectroscopy), Hetero COSY (^{1}H,^{13}C COSY,HMQC), long range ^{1}H,^{13}C COSY (HMBC), NOESY and 2D-INADEQUATE experiments and their applications.

2. Optical Rotatory Dispersion (ORD) and CD Spectroscopy: Optical rotation, circular birefringence, circular dichroism and Cotton effect. Plain curves and anomalous curves and their applications in determining configuration and in study of conformational changes. Empirical and semiempiricaj rules-The axial haloketone rule, the octant rule, Helicity rule, Exciton chirality method-Exciton coupling between identical chromophores. Benzene sector and chirality rule. Application to the study of absolute configuration and conformations of organic molecules.

PO-27: Pericyclic reactions I **(15 Hrs)**

Introduction - Characteristics and classification of pericyclic reactions— Electrocyclic, cycloaddition & cycloreversions and sigmatropic reactions—4ne and 4n+2e type examples.

Approaches for the interpretation of mechanism of pericyclic reactions- Aromatic Transition States (ATS)/Perturbation Molecular Orbitals (PMO) approach-Concept of Huckel –Mobius aromatic and antiaromatic transition states. Framing Woodward-Hofmann selection rules for all the pericyclic reactions by ATS approach. Solving problems based on ATS approach.

Aromaticity: Aromatic and anti aromatic compounds. Criteria for aromaticity. Huckel's 4n+2 electron rule for benzene and non benzenoid aromatic compounds. Eg. Cyclopropenium ion, cyclopentadienyl ion, cycloheptatrienium ion, azulene and annulenes.

PO-28: Pericyclic reactions II **(15 Hrs)**

Molecular orbitals-definition and their origin-Non-mathematical writing up of molecular orbitals and their symmetry properties for acyclic conjugated systems. Frontier Molecular Orbital (HOMO-LUMO) approach-concept-Framing Woodward-Hofmann selection rules for all the pericyclic reactions by Frontier Molecular Orbital (FMO) approach. Solving problems based on FMO approach.

Conservation of orbital symmetry (Correlation Diagrams) approach-concept-Framing Woodward-Hofmann selection rules for electrocylic and cycloadditions & cycloreversions by Conservation of orbital symmetry approach.

Recommended Books :

1. Spectroscopic identification of organic compounds by RM Silverstein, G C Bassler and T B Morrill.
2. Organic Spectroscopy by William Kemp.
3. Spectroscopic methods in Organic chemistry by DH Williams and I Fleming.
4. Modern NMR techniques for chemistry research by Andrew B Derome.
5. NMR in chemistry - A multinuclear introduction by William Kemp.
6. Spectroscopic identification of organic compounds by P S Kalsi.
7. Introduction to organic spectroscopy by Pavia.
8. Carbon-13 NMR for organic chemists by GC Levy and O L Nelson.
9. Nuclear Magnetic Resonance Basic principles by Atta-ur-Rahman.
10. Advanced organic chemistry. Part A Structure & Mechanism by Francis A. Corey and Richard J. Sundberg.
11. Optical rotatory dispersion by C Djerassi.

12. Optical rotatory dispersion and circular dichroism by P Crabbe.
13. Mechanism and Structure in Organic chemistry by S Mukherjee.
14. Advanced Organic Chemistry: Reactions, Mechanisms & Structure by Michael B Smith & Jerry March.
15. Pericyclic Reactions by Mukherjee S M.
16. Conservation of Orbital Symmetry by Woodward and Hoffmann.
17. Organic Reactions and Orbital Symmetry, Gilchrist and Storr.
18. Pericyclic Reactions — a problem solving approach, Lehr and Merchand.
19. The Nature of Chemistry — Units 17-19 - Aromaticity — Open University, U K. Publications.
20. The aromaticity III level, units 17-19 British open university volumes.
21. Aromatic character and aromaticity by G.M.Badger.
22. Non-benzenoid aromatic compounds by D.Ginsberg.
23. Nonbenzenoid compounds by Lloyds.

CHOICE BASED (CB) PAPERS

Paper-IV

CH (PO) 404T(CB_1): Heterocyclics , Biomolecules, Green chemistry and Principles of Drug design and discovery

PO-(CB_1)- 29: Five and six membered heterocyclics with two hetero atoms
PO-(CB_1)- 30: Biomolecules
PO-(CB_1) - 31: Green chemistry
PO-(CB_1) - 32: Principles of Drug design and drug discovery

PO-(CB_1)-29: Five and six membered heterocyclics with two hetero atoms (15 Hrs)

Synthesis, reactivity, aromatic character and importance of the following heterocycles: Pyrazole, Imidazole, Oxazole, Thiazole, Isoxazole, Isothiazole, Pyridazine, Pyrimidine. Pyrazine, Oxazine thiazine, benzimidazole, benzoxazole and benzthiazole.

PO-(CB_1)- 30 : Biomolecules (15 hrs)

1. Enzymes: Definition. Classification based on mode of action. Mechanism of enzyme catalysis. Lock and Key model and Induced- Fit model. Enantiomer discrimination by Three- point Contact model. Factors affecting enzyme catalysis.Enzyme inhibition- reversible and irreversible inhibition. Enzymes in organic synthesis. Immobilised enzymes.

2. Nucleic acids: Primary, secondary and tertiary structure of DNA. Types of mRNA,tRNA and rRNA. Replication, transcription and translation. Genetic code. Protein biosynthesis. Chemical Synthesis of nucleosides and nucleotides.

3. Lipids: Lipid structure- acylglycerols, phosphoglycerides and sphingolipids. Biosynthesis of Lipids and chemical Synthesis of lipids.

PO-(CB_1)-31: Green Chemistry (15Hrs)

Introduction: Principles, atom economy and scope. Introduction to alternative approaches.

1. Solvent free reactions-principle, scope, utility of solvent free condition reactions.
Organic Synthesis in solid state (without using any solvent): Michael addition, Beckmann rearrangement, Synthesis of aziridines; solid supported organic synthesis: Synthesis of aziridines, pyridines, chromenes and flavones.
2. Aqueous Phase Reactions: Diels-Alder Reaction, Heck reaction, epoxidation,Dihydroxylation (Syn- & Anti-)
3. Microwave Technology: Microwave equipment, activation-benefits, limitations, microwave effects.
a) Microwave Solvent free reactions (Solid state Reactions) - Deacetylation, deprotection, saponification of esters, alkylation of reactive methylene compounds, synthesis of nitriles from aldehydes, reductions.
b) Microwave assisted reactions in water — Hoffmann elimination, hydrolysis, oxidation, saponification reactions.
c) Microwave assisted reactions in organic solvents — Esterification reactions, Fries rearrangement, Orthoester Claisen rearrangement, Diels- Alder reaction, decarboxylation.
d) Microwave assisted reactions under PTC conditions:
4. Ultrasound assisted reactions: introduction, substitution reactions, addition, oxidation, reduction reactions.
5. Organocatalysis: Aldol reactions, Acyl transfer reactions, nucleophilic N-heterocyclic carbenes in asymmetric organocatalysis, setter reaction and Baker's Yeast.
6. Ionic liquids: Introduction and applications in organic synthesis (illustrate with two examples).

PO-(CB_1)- 32: Principles of Drug design and discovery 15 Hrs

Introduction to drug discovery. Folklore drugs, stages involved in drug discovery- disease, drug targets, bioassay. Discovery of a lead- screening of natural products and synthetic compound libraries. Existing drugs as leads (me too drugs). Pharmacokinetics (ADME), pharmacodynamics. Nature of drug – receptor interactions and their theories – Occupancy theory, Induced – fit theory, Macromolecular purturbation theory and Two-state model of receptor activation. Natural products as lead structures in drug discovery – Pharmacophore - structure pruning technique e.g. morphine. Discovery of lead structure from natural hormones and neurotransmitters. Principles of design of agonists (e.g.Salbutamol), antagonists e.g. cimitidine) and enzyme inhibitors (e.g. captopril). Drug discovery without lead – serendipity- Penicillin and Librium as examples. Principles of prodrug design. Introduction to drug patents and Clinical trials.

Recommended Books

1. Heterocyclic Chemistry, T.Gilchrist.
2. An introduction to the Chemistry of heterocyclic compounds, R.M.Acheson.

3. Heterocyclic Chemistry, J.A.Joule & K.Mills.
4. Principles of Modern Heterocyclie Chemistry, A.Paquette.
5. Heterocyclic Chemistry, J,A.Joule & Smith.
6. Handbook of Heterocyclic Chemistry, A.R.Katritzky.
7. Enzyme structure and mechanism by Fersht and Freeman
8. Bio-Organic chemistry by Hennan Dugas
9. Nucleic acids in Chemistry and Biology by G M Blackbum MI Gait
10. Lehninger Principles of Biochemistry by D L Nelson and M M Cox
11. Outlines of Biochemistry by Conn and Stumpf
12. Biotransformations in Organic Chemistry by K Faber.
13. Green chemistry, Theory and Practical, Paul T.Anastas and John C.Warner.
14. New trends in green chemistry By V.K.Ahulwalia and M.Kidwai.
15. Organic Synthesis: Special techniques. V.K.Ahulwalia and Renu Aggarwal.
16. Burger's medicinal chemistry and drug discovery by Manfred E. Wolf.
17. Introduction to Medicinal chemistry by Patrick.
18. Introduction to drug design by R Silverman
19. Comprehensive medicinal chemistry. Vol 1-5 by Hanzsch.
20. Principles of medicinal chemistry. by William Foye

Paper-IVCH (PO) 404T(CB_2): Modern material Chemistry & Combinatorial Chemistry

PO-(CB_2)-29: Types of materials, Conducting Organics and NLO materials
PO-(CB_2)-30: Functional Polymers
PO-(CB_2)-31: Dynamics of biopolymers
PO-(CB_2)-32: Combinatorial Chemistry

PO-(CB_2)-29: Types of materials, Conducting Organics and NLO materials (15 hrs)

Classification of materials – metals, ceramics, polymers, composites, semiconductors and biomaterials. Glassy state – glass formers and glass modifiers, applications
Ceramics – criteria for determining the crystal structure of ceramic materials – examples. Mechanical properties of ceramics. Composites – particle reinforced and fiber reinforced composites. Preparative methods of solid materials. Ceramic method – coprecipitation, sol-gel, high pressure and hydrothermal methods – Arc technique.
Techniques of single crystal growth – growth from solutions – growth from melts – growth from vapor.
NLO materials – basic concepts, second and third harmonic generation, examples of organic, inorganic and polymer nlo materials.
Conducting organics – Fullerenes, alkali metal doped fullerides, fullerenes as superconductors

PO-(CB_2)-30: Functional Polymers (15hrs)

Smart materials – their uses in sensing devices and communication networks.
Conducting polymers. Electrically conducting polymers and their uses (polyanilines, polypyrrole, polyacetylene and polythiophene). Photoconductive polymers. Liquid crystal polymers – smectic, nematic and cholesteric structures.
Ionic exchange polymers. Cationic and anionic exchange polymers and their uses. Eco-friendly polymers.
Membrane separation. Filtration – micro, ultra and nanofiltration. Separation of gases – permeselectivity and gas permeability of representative polymers. Liquid separation – dialysis, electro osmosis and reverse osmosis. Fire retarding polymers, photonic polymers.
Polymers in biomedical applications – artificial organs and controlled drug delivery.

PO-(CB_2)-31: Dynamics of biopolymers (15 hrs)

Biolpolymer interactions. Basic principles of molecular mechanics. Molecular potentials. Bonding and nonbonding potentials. Electrostatic interactions, dipole-dipole interactions and van der Waals interactions. Hydrogen bonds.

Protein structure. Stabilizing interactions in proteins. The Corey-Pauling rules. The α-helix and the β-sheet. Conformational energy. Potential energy diagrams and Ramachandran plots.

Chain configuration of macromolecules. Random linear structure of biopolymers. Random walk. Random coils and measures of size – the contour length, the rms separation and the radius of gyration. Conformational entropy. Introductory treatment of the protein folding problem.

PO-(CB_2)-32: Combinatorial Chemistry (15Hrs)

Introduction. Combinatorial approach. Combinatorial libraries, technologies. Solid phase synthesis, requirements-resins. Linkers. Reactants for solid phased synthesis. Methods of Parallel synthesis: Haughton's tea bag procedure. Automated parallel synthesis. Methods in Mixed combinatorial synthesis: general principles. Furkas mix and split combinatorial synthesis, Structure determination of active compounds-Deconvolution, Methods in deconvolution-recursive deconvolution, tagging and use of decoded sheets. Examples of Combinatorial Chemistry. Planning and designing of combinatorial synthesis, Spider leg scaffolds, drug molecules. Automation in Combinatorial chemistry. High throughput screening.

Recommended Books

1. Introduction to Chemical reaction Engineering and Kinetics, R. W. Missen, C. A. Mims & B. A. Saville, John Wiley.
2. Chemical Reaction Engineering, O. Levenspiel, John Wiley.
3. Chemical Engineering Kinetics, J. M. Smith, McGraw Hill.
4. New directions in solid state chemistry. CNR Rao and Gopalakrishnan.
5. Principles of the Solid State, H. V. Keer, New Age International.
6. Material Science and Engineering – An Introduction, William D. Callister, Jr., John Wiley & Sons.
7. Biophysical Chemistry, Cantor & Schimmel, W. H. Freeman and Company.
8. Principles of Physical Biochemistry, Kensal E van Holde, W. Curtis Johnson & P. Shing Ho, Prentice Hall.
9. Physical Biochemistry : Principles and Applications, David Sheehan, John Wiley.

10. Physical Chemistry for the Chemical and Biological Sciences, Raymond Chang, University Science Books.
11. Materials Science & Engineering – A First Course, V. Raghavan, Prentice Hall.
12. Medicinal chemistry An introduction by Garreth Thomas
13. Medicinal Chemistry by G. Patrick.

Paper-IV CH (PO) 404T(CB_3): Bioplymer chemistry

PO-(CB_3)- 29: Bioenergetics & physical properties of biopolymers
PO-(CB_3)- 30: Biological membranes & binding of ligands by biopolymers
PO-(CB_3) - 31: DNA, genes & cloning
PO-(CB_3) - 32: Bioinformatics

PO-(CB_3)- 29: Bioenergetics & physical properties of biopolymers (15 hrs)

Bioenergetics. The standard state in biological processes. ATP – the currency of energy. Gibbs energy change in ATP hydrolysis, comparison with other phosphates. Principles of coupled reactions. Glycolysis and coupled reactions involving ATP. Biological oxidation-reduction reactions – transfer of H^+ ions and electrons. Synthesis of ATP in the mitochondria. The chemiosmotic theory. Gibbs energy change accompanying the proton movement.
Viscometry. Molecular weights. Use of viscometry in the study of ligand binding to DNA. Separation/molecular weight studies of biopolymers.Light scattering method.
Sedimentation. Sedimentation velocity. Sedimentation coefficient. The Sverdberg equation. Sedimentation equilibrium analysis. Ultra centrifugation Molecular weights. Light scattering method.
Electrophoresis – principle involved. Gel electrophoresis. Electrophoretic mobility. Applications.

PO-(CB_3)- 30: Biological membranes & binding of ligands by biopolymers (15 hrs)

Structure and function of cell membrane. Membrane equilibria and thermodynamics of membrane equilibria. Dialysis equilibrium. Osmotic pressure. Membrane potentials. Transport across membranes. Passive transport, facilitated transport and active transport Sodium-potassium pump. Selective ion transport and membrane potential. The Goldman equation (derivation not required). Nerve cells. The transfer of information in the body. The action potential and the mechanism of action potential propagation. Signal transducing mechanism involving gated ion channels in the plasma membrane.
Binding of ligands and metal ions to macromolecules – one and n-euqivalent binding sites per molecule. Allosteric interactions – Oxygen binding to myoglobin and hemoglobin – Cooperative and non-cooperative binding. Hill equation and Hill plots. Transport of H^+ and CO_2 . Bohr effect.

PO-(CB_3) - 31: DNA, genes & cloning (15 hrs)

Watson –Crick model of DNA. Types of DNA chains – linear, circular and supercoiled DNA. Types of RNA. Secondary structure of t-RNA. Genes and genome. Gene expression. Transcription and translation (general principles only). Codons and the genetic code.
Sequence analysis of DNA by the Sanger chain-termination method.
Introduction to biotechnology and recombinant DNA technology. Molecular cloning. Restriction endonucleases and cloning vectors. Steps involved in the construction of recombinant DNA. DNA hybridization and hybridization probes.
Satellite DNAs – micro and mini satellites. Sequence polymorphisms – RFLPs. Principles of DNA finger printing technology.

PO-(CB_3) - 32: Bioinformatics : (15 hrs)

Introduction: Use of informatics and computers in biology.
Homology as descendants of common ancestors, statistical analysis of sequence alignment. General purpose Databases for Comparative Genomics: COGs, KEGG, MDGB - Organism Specific Databases examples - E. Coli, Yeast, Oryza.
Introduction to Proteins - primary, secondary, tertiary and quaternary structures. Structure databases – PDB, MMDB, CSD. Homology modeling – Flow chart, structure refinement - Ramachandra Plot.

Books suggested:

1. Biophysical Chemistry, Cantor & Schimmel, W. H. Freeman and Company
2. Principles of Physical Biochemistry, Kensal E van Holde, W. Curtis Johnson & P. Shing Ho, Prentice Hall
3. Physical Biochemistry : Principles and Applications, David Sheehan, John Wiley
4. Physical Chemistry for the Chemical and Biological Sciences, Raymond Chang, University Science Books
5. Lehninger Principles of Biochemistry, D. L. Nelson & M. M. Cox, MacMillan
6. Biochemistry, L. Stryer, W. H. Freeman and Company
7. Concepts in Biochemistry, Rodney Boyer, Books/Cole Publishing Company
8. Modern Electrochemistry 2B, Bockris & Reddy, Kluwer Academic/ Plenum
9. Introduction to Bioinformatics by Arthur Lesk, Oxford University Press, Inc, New York
10. Bioinformatics , A practical guide to the Genes and Proteins. Edited by Andreas. D. Baxevanis and B. F. Francis Wley Puublishers

SEMESTER IV LABORATORY COURSES

PAPER VII

(Lab)-CH(PO) 451P: Instrumentation

I. Conductometry: 1. Conductometric titrations :

- Mixture of strong and weak bases vs strong acid
- Mixture of strong and weak bases vs weak base
- Mixture of strong acid, weak acid and CuSO4 vs strong base
- Formic acid, acetic acid, chloro acetic acid, dichloro acetic acid and trichloro
- acetic acid and their mixtures vs strong base
- Precipitation titration: K_2SO_4 vs $BaCl_2$

2. Dissociation constant of weak acids
3. Effect of solvent dielectric constant on dissociation constant of a weak acid
4. Verification of Onsager equation
5. Composition of CU(II)-tartaric acid complex by Job's method

II. pH – metry:

1.Preparation of a) phosphate b) acetate & c) borate buffers
2. pH-metric titrations of
a) monobasic acids vs strong base b) dibasic acids vs strong base
c) tribasic acids vs strong base d) mixture of strong and weak acids vs strong base
3.Determination of dissociation constant of monobasic/dibasic acids by Alber-Serjeant method.
4. Determination of dissociation constant of acetic acid in DMSO, acetone and dioxane.
5. Determination of pKa and pKb of glycine(calculation using a computer program)
6. Determination of stability constant of a metal complex.

III, Spectrophotometry:

1.Estimation of a) Cu(II) using EDTA b) Fe(III) using thiocyanate
c) Fe(II) using 1,10-phenanthroline
d) Fe(III) in tap water using thiocyanate by standard addition method
e) Simultaneous determination of dichromate and permanganate in a mixture
2. Spectrophotometric titrations: a) Cu(II) vs EDTA b) Fe(II) using 1,10-phenanthroline
3. Determinaton of composition of
a) Cu(II)-EDTA complex by Job's method
b) Fe(II)-phenanthroline complex- by Job's method by mole ratio method and by slope ratio method
4. Determination of composition and Gibbs energy of formation of -
Fe(III)-salicylic acid complex

5..Determination of pKa of methyl red indicator

IV Potentiometry: 1.Potentiometric titrations :

a. Weak acid vs strong base and calculation of dissociation constants
b. Mixture of strong and weak acids vs strong base
c. Dibasic acid vs strong base
d. Fe(II) vs Ce(IV) and calculation of formal redox potentials of Fe(II)/Fe(III)
e. Fe(II) vs EDTA
f. Mixture of halides vs $AgNO_3$
g. Mixture of KI and KSCN vs $AgNO_3$

V. Polarography - Determination of Pb^{2+}, and Ni^{2+} separately.

Suggested Books:

1. The systematic identification of organic compounds by R L Shriner, R C Fusion and D Y Curtin
2. A textbook of practical organic chemistry by A I Vogel, Vol I & II
3. Unitized experiments in organic chemistry by R Q Brewster and others
4. Handbook of organic analysis by HTC Clarke
5. Practical Organic Chemistry by Mann and Saunders
6. Spectroscopic identification of organic compounds by Silverstein , Bassler & Morrel.

Paper VIII
(LAB) CH (PO) 452P : Separation & identification and spectral analysis

1. Separation of two component mixtures by chemical methods and their identification by chemical reactions – separation by using solvent ether , dil. hydrochloric acid , 5% aqueous sodium bicarbonate and sodium hydroxide solutions, checking the purity of the two components by TLC , identification of the compounds by a systematic study of the physical characteristics (mp/bp) , extra elements (nitrogen , halogens and sulfur) , solubility , functional groups , preparation of crystalline derivatives and identification by referring to literature. A minimum of 6 mixtures should be separated and analyzed by these procedures.
2. Separation of three component mixtures by chemical method. A minimum of 2 mixtures should be separated.
3. Identification of unknown organic compounds by interpretation of IR, UV, 1H nmr, 13C nmr and mass spectra. A minimum of 30 representative examples should be studied.

Suggested Books:

1. The systematic identification of organic compounds by R L Shriner, R C Fusion and D Y Curtin
2. A textbook of practical organic chemistry by A I Vogel, Vol I & II
3. Unitized experiments in organic chemistry by R Q Brewster and others
4. Handbook of organic analysis by HTC Clarke
5. Practical Organic Chemistry by Mann and Saunders
6. Spectroscopic identification of organic compounds by Silverstein , Bassler & Morrel.

ANALYTICAL CHEMISTRY SPECIALISATION

SYLLABUS (2012 – 13) ONWARDS

III & IV SEMESTERS

M.Sc. CHEMISTRY(ANALYTICAL CHEMISTRY)

FOR STUDENTS ADMITTED IN THE YEAR (2011 – 12)

REVISED AS PER NEW (CB) SYLLABUS

M.Sc. CHEMISTRY(ANALYTICAL CHEMISTRY)

Syllabus for III and IV Semesters

(For the batch admitted during the academic year 2011-2012 under the CBCS pattern)

[Under Restructured CBCS Scheme]

(Approved in the P.G. BOS meeting held on 15-9-2012)

Semester - III

	Instruction	Internal assessment	Semester exam*	Total	Credits
	Hrs/week	**marks**	**marks**	**marks**	
CH(AC) 301T	4	20	80	100	4
CH(AC) 302T	4	20	80	100	4
CH(AC) 303T	4	20	80	100	4
CH(AC) 304T	4	20	80	100	4
SEMINAR	2	--	--	25	1
CH(AC) 351P	9	--	100	100	4
CH(AC) 352P	9	--	100	100	4
Total				**625**	**25**

*Theory: 3 hours; Practical's: 6 hours

Semester - IV

	Instruction	Internal assessment	Semester exam*	Total	Credits
	Hrs/week	**marks**	**marks**	**marks**	
CH(AC) 401T	4	20	80	100	4
CH(AC) 402T	4	20	80	100	4
CH(AC) 403T	4	20	80	100	4
CH(AC)404T (CB)	4	20	80	100	4
SEMINAR	2	--	--	25	1
CH(AC) 451P	9	--	100	100	4
CH(AC) 452P	9	--	100	100	4
Total				**625**	**25**

(**Choice based paper (CB) =** Paper offered by the same Department or other Department in the Science faculty)

*Theory: 3 hours; Practical's: 6 hours

Grand total (all 4 semesters), 2500 marks and 100 credits

M.Sc Chemistry(Analytical Chemistry)

Semester III

Paper- I: CH (AC) 301T: Sampling, Data handling, Classical and Atomic spectral methods of analysis
AC – 01 Sampling & Data handling
AC – 02 Titrimetric & Gravimetric analysis
AC – 03 Thermal & Radiochemical methods of analysis
AC – 04 Atomic Spectroscopy

Paper-II: CH (AC) 302T: Spectroscopic methods of Analysis-I
AC – 05 Multinuclear NMR
AC – 06 Advanced NMR
AC – 07 Electron Spin Resonance Spectroscopy
AC – 08 Mossbauer and NQR

Paper-III: CH (AC) 303T: Spectroscopic methods of Analysis-II
AC – 09 U.V. visible spectroscopy,
AC –10 IR & Raman spectroscopy
AC – 11 Optical Methods
AC – 12 Fluorimetry, Phosphorimetry, Nephelometry and Turidimetry

Paper-IV: CH (AC) 304T: Separation Methods
AC-13 Solvent extractions
AC –14 Chromatography
AC – 15 Mass spectrometry & Hyphenated techniques
AC – 16 Electrophoresis

LABORATORY COURSE
Paper CH (AC) 351P: Titrimetry, Solvent extraction,Chromatography and Water analysis.

Paper CH (AC) 352P: Colorimetry, Spectrophotometry

Semester IV

Paper-I CH (AC) 401T: Miscellaneous Methods of Analysis

AC – 17 Surface Analysis Methods
AC – 18 Diffraction Methods, X-Ray Absorption and X-Ray Fluorescence
AC –19 Electroanalytical Methods
AC – 20 Micromeritics, Dissolution and disintegration

Paper -II CH(AC) 402T:Applied Aalysis
AC –21 Industrial Analysis
AC –22 Analysis of Air and Water Pollutants
AC – 23 Clinical and Pharmaceutical analysis
AC – 24 Food and Agricultural analysis

Paper-III CH (AC) 403T: Laboratory Management
AC – 25 Automation in laboratory
AC – 26 LIMS & Computer aided analysis
AC – 27 Laboratory Management & Standard reference materials
AC – 28 Accreditation of Laboratories, Quality management

PAPER – IV: CHOICE BASED PAPER -1
CH (AC)(CB_1) 404 : Quality Assurance and Accreditation
AC(CB_1) -1 Quality Assurance – I
AC(CB_1) -2 Quality Assurance – II
AC(CB_1) -3 Quality Assurance – III
AC(CB_1)- 4 Quality Accreditation

PAPER – IV: CHOICE BASED PAPER -2
CH (AC)(CB_2) 404T : Applied analysis and Green Analytical Chemistry
AC(CB_2) -1 Enzyme catalysis- Analytical applications
AC(CB_2) -2 Forensic Chemical Analysis
AC(CB2) -3 Limit tests
AC(CB_2)- 4 Green Analytical Chemistry
LABORATORY COURSE
Paper CH (AC) 451P: Electro analytical techniques:

Paper CH (AC) 452P: Spectroscopy and Evaluation of Physical Parameters Of Tablets

M.Sc. CHEMISTRY(ANALYTICAL CHEMISTRY)
Syllabus for III and IV Semesters
(for the batch admitted during the academic year 2011-2012 under the CBCS pattern)
[Under Restructured CBCS Scheme]
III Semester Syllabus
Paper- I:

CH (AC) 301T: Sampling, Data handling, Classical and Atomic spectral methods of analysis

AC – 01 Sampling & Data handling
AC – 02 Titrimetric & Gravimetric analysis
AC – 03 Thermal & Radiochemical methods of analysis
AC – 04 Atomic Spectroscopy

AC – 01 Sampling & Data handling 15 Hrs

Classification of Analytical Methods. Types of samples, Preparation of sample for analysis, effect of sampling uncertainties, sample treatment, moisture in sample, decomposition of organic & inorganic compounds, procedure of sampling of solids, liquids and gases.

Errors and Evaluation:-Accuracy, precision, sensitivity, detection limits, significant figures, rounding off. Types of errors – determinate and indeterminate errors. Ways of expressing accuracy, absolute and relative errors. Significant figures and propagation of errors. Confidence limit, Test of significance – the F-test and T-test. The statistical Q-test for rejection of a result, statistics for small data sets. Linear least squares method. The correlation coefficient. Calculation for the above parameters.

AC – 02 Titrimetric and Gravimetric Analyses 15 Hrs

Redox titrations: Formal and Standard potentials in various media, standardization, Oxidizing systems: Mn(VII), Ce(IV), Cr(VI). V(V). Reducing systems: V(II), Ti(III), Sn(II), Fe(II) in H_3PO_4. Detection of end point in redox titrations – selection of suitable indicator.

Complexometric titrations: Introduction, stability constants of EDTA complexes, titration curves, types of EDTA titrations with examples. Standard EDTA solutions, some practical considerations during EDTA titrations. Titration of mixtures (Mg^{2+}&Ca^{2+}; Pb^{2+}&Ca^{2+}; Mn^{2+}&Mg^{2+}), selectivity, masking and demasking agents. Metal ion indicators: General properties, theory of the use of metal ion indicators, use of Murexide, Eriochrome black - T, Calcon, Xylenol orange, Methyl thymol blue, Fast sulphon black - F.

Gravimetric Analysis: Theory, principles, precipitation reagents (DMG, Oxine), Determination of Nickel as dimethylglyoximate, Aluminium as 8-hydroxyquinolate & Chloride as silver chloride.

AC – 03 Thermal and Radiochemical methods of Analysis 15 Hrs

Thermal methods of analysis: Thermogravimetry, Differential Thermal Analysis and Differential Scanning Calorimetry, instrumentation. Methodology of TG, DTA and

DSC.Thermomechanical analysis, Dynamic mechanical analysis. Application of TG to study of oxalates and chromates. Determination of Glass transition, Heat capacity determination, Characterization of polymer blends. Problems based on decomposition path way and % composition. Evolved gas analysis.
Thermometric titrimetry – theory, instrumentation, applications.
Radiochemical methods of analysis: Radioactive tracer techniques and its applications, isotope dilution analysis, neutron activation analysis, radiometric titrations: principle, theory, applications and problems.

AC – 04 Atomic Spectroscopy 15 Hrs

Atomic Absorption Spectroscopy (AAS): Principles of AAS, Instrumentation – flame AAS and furnace AAS, resonance line sources, sensitivity and detection limits in AAS, interferences –chemical and spectral, evaluation methods in AAS and applications in qualitative and quantitative analysis.
Atomic Emission Spectroscopy (AES): Principle of AES, Instrumentation, evaluation methods, Application in quantitative analysis.
Inductively Coupled Plasma- Atomic Emission Spectroscopy (ICP-AES): Limitations of AES, Principles of plasma spectroscopy, plasma as an excitation source. Inductively coupled plasma source, ICP-AES – Instrumentation. Applications of ICP-AES.Comparison with AAS.

Suggested Books

1. Principles of Instrumental Analysis - Skoog, Holler, Nieman, 5th ed., Harcourt College Publishers, 1998.
2. Analytical Chemistry – Gary D. Christian, 6th ed., John Wiley and sons. Inc., New York 1994.
3. Instrumental methods of Analysis - Willard, Merit, Dean, 6th ed., CBS Publishers & distributors, 1986.
4. Hand Book for Instrumental Techniques for Analytical Chemistry, Ed. Frank Settle, Prentice Hall, New Jersey, USA, 1997.
5. Vogel's Text book of Quantitative Analysis – GJ Jeffery, J Bassett et al, 5th ed., Longmann, ELBS Publications, 2000.
6. Principles and practice of Analytical Chemistry, F.W.Fifield & D Kealey, 5th Ed. Blackwell Science, 2000.
7. Quantitative Chemical Analysis, Daniel C. Harris, 6th Ed. WH Freeman & Co. NewYork, 2003.
8. Analytical Chemistry An Introduction, Crouch, 7th Ed. Saunders College Publishing,2000.
9. Organic Analytical Chemistry theory and practice, Jag Mohan, Narosa Publications,2003.
10. Pharmaceutical analysis,. Watson
11. Electronic Absorpption Spectroscopy and related techniques, D.N.Satyanarayana, University Press, 2001.

Paper-II:

CH (AC) 302T: Spectroscopic methods of Analysis-I

AC – 05 Multinuclear NMR
AC – 06 Advanced NMR
AC – 07 Electron Spin Resonance Spectroscopy
AC – 08 Mossbauer and NQR

AC – 05 Multinuclear NMR

^{13}C nmr spectroscopy: CW and PFT techniques. Types of 13C nmr spectra: undecoupled, proton- decoupled, single frequency off-resonance decoupled (SFORD) and selectively decoupled spectra. ^{13}C chemical shifts, factors affecting the chemical shifts

Chemical equivalence and magnetic equivalence. Virtual Coupling and its importance in study of Metal Complexes $[Pd\{P(CH_3)_3\}_2I_2]$. Spin Dilute Systems-Satellites in Pt(II) Complexes cis-$[Pt(PEt_3)_2Cl_2]$, $Sn(CH_3)_4$. NMR Time Scale and its use in studying Stereo chemical Non –rigidity (PF_5, $[Rh(PR_3)_5]^+$, $[Rh\{Cp\}_2(CO)_2]$) -ΔR, the Ring Contribution to ^{31}P Chemical Shifts –Metal and Chelate size on ΔR. Applications of ^1H, ^{13}C, ^{19}F, ^{31}P and ^{15}N to simple inorganic and Coordination Compounds - 1)^1H-NMR: $PtHCl(PEt_3)_2$, $Pt(NH_3)_3(CH_3)_3$, BH_4^-, NH_4^+, CH_3CN, [^{6}h- C_7H_8 $Mo(CO)_3$], [^{7}h-$C_7H_7Mo(CO)_3]^+$, B_2H_6; $^{29}SiH_3SiH_3$, 2)^{19}F: BF_4^-, H_2PF_3; 3)^{31}P: $Mo(CO)_3(PPh_3)_3$, [Rh $(PPh_3)_3Cl$] ,trans-$[PtCl_4(PEt_3)_2]$, $^{31}PF_2H(^{15}NH_2)_2$ 4) 13C; [^{4}h C_8H_8 $Ru(CO)_3$], $Fe(CO)_5$, $Fe_2(CO)_9$, $Fe_3(CO)_{12}$, $FeICp(CO)_2$, $Cl(CH_2)_3Si(OCH_3)_3$, [$^{13}C^{15}N$ $Co(DH)_2$Pyridine]. $^{13}C\{^1H\}$ NMR spectrum of σ-bonded C_6H_5 ligand

AC – 06 Advanced NMR Spectroscopy: - Spin-Lattice (T_1) and Spin-Spin Relaxation (T_2). pin Echo Polarization Transfer – Spin Echo Measurements. ^{13}C-NMR spectral editing techniques: Attached proton test (APT spectra) by Gated Spin Echo, Cross polarization, INEPT spectra, DEPT spectra (Distortionless enhancement by polarization transfer) (eg $Cl(CH_2)_3Si(OCH_3)_3$). INADEQUATE spectra (Incredible Natural Abundance Double Quantum Transfer Experiment).

Two Dimensional NMR: Basic principles, Types of 2-D NMR ;i)J- resolved spectroscopy a)homo and b)Heteronuclear J- resolved spectroscopy ii) Correlation spectroscopy ; Homo nuclear shift correlation spectroscopy (COSY) and Hetero nuclear shift correlation spectroscopy (HETCOR) iii) NOESY(Nuclear Overhauser Enhancement Spectroscopy). HOESY (two dimensional heteronuclear NOE). Advantages of 2-D NMR

AC – 07 Electron Spin Resonance Spectroscopy

Principle- Selection Rules – Instrumentation- Microwave source(energy bands). Application of ESR to the study of simple free radicals: methyl (CH_3)., amine (NH_2)., diphenyl picryl hydrazyl, cyclopentadienyl (C_5H_5)., hydroxy methyl(CH_2OH).radicals. Zero-Field Splitting (ZFS) - Effective Spin - Orbitally Non-degenerate and Degenerate States. ESR Spectra of d^1-d^9 Transition Metal Complexes with examples. Interpretation of g in cubic ,axial and rhombohedral geometries. Factors affecting g values. Calculation of g values with

simple examples. Intensities of '$g_{\parallel}$ and $g^{\perp}$ peaks . Evidence for Metal-Ligand Bond Covalency- Cu(II)- Bis –Salicylaldimine. $[(NH_3)_5\,Co\,O_2\,Co\,(NH_3)_5]^{5+}$, Cu(II)- diethyldithio phosphinate, Vanadyl dithio phsphinate, Copper(II) tetraphenyl porphyrin, Co(II)-phthalocyanine, $K_2[IrCl_6]$. Interpretation of 'g' and 'A' values from esr spectral data in- i) MnF_6^{4-}, ii) CoF_6^{4-}, and CrF_6^{3-}. ESR spectra of dinuclear Cu (II) complexes.

AC – 08 Mossbauer and Nuclear Quadrupole Resonance Spectroscopy

Mossbauer Spectroscopy :Principle, Experimental Considerations and Presentation of the Spectrum - Isomer Shifts – Quadrupole splitting and Magnetic hyperfine splitting - Selection Rules.

Applications

Iron Compounds: Low-spin and High-spin Fe(II) and Fe(III) Complexes - π-bonding Effects in Iron complexes - Study of High-spin Low-spin Cross-over c) Diamagnetic and Covalent Compounds - Structural aspects of Iron Carbonyls and Iron-Sulfur Proteins

Tin Compounds: Tin Halides and Organotin Compounds.

Iodine Compounds: Isomer Shifts of ^{127}I and ^{129}I – Applications to Alkali metal iodides and Molecular Iodine. .

Nuclear Quadrupole Resonance Spectroscopy : Principle, nuclear quadrupole resonance experiment, structural information from NQR spectra, Interpretation of nuclear quadrupole coupling constants.

SUGGESTED BOOKS

1. Structural Methods in Inorganic Chemistry, E. A. V. Ebsworth, D. W. H. Rankin and S. Craddock, ELBS.
2. Physical Methods in Chemistry, R. S. Drago, W.B. Saunders Co., 1977.
3. Physical Methods for Chemists, Russell S. Drago Second edition, Saunders College Publishing, 1992.
4. Principles of Mossbauer spectroscopy, T. C. Gibb, Chapman and Hall, London, 1976.
5. Mossbauer Spectroscopy, N. N. Greenwood and T. C. Gibb, Chapman and Hall, London, 1971.
6. Principles of Instrumental Analysis, Skoog, Holler and Nieman.
7. Instrumental Techniques for Analytical Chemistry, Frank Settle.
8. Principles of Analytical Chemistry, M. Valcarcel.
9. Physical Methods in Advanced Inorganic Chemistry, Hill and Day
10. Magneto Chemistry, Dutta & Shyamal
11. Oxford Chemistry Primers, Vol 62

Paper-III

CH (AC) 303T: Spectroscopic methods of Analysis-II

AC – 09 U.V. visible spectroscopy,

AC –10 IR & Raman spectroscopy

AC – 11 Optical Methods

AC – 12 Fluorimetry, Phosphorimetry, Nephelometry and Turidimetry

AC – 09: UV and visible spectroscopy 15 Hrs

UV and visible spectroscopy : Beer Lamberts law, Real limitations to Beer's law,instrumentation for colorimetry and spectrophotometry – Numerical problems based on Beer's law, simultaneous & differential spectrophotometry. First derivative spectrophotometry. Classification of Electronic Spectra for Metal Complexes, Selection Rules: Electric Dipole Transitions, Magnetic Dipole Transitions, Orbital Selection Rules, Spin Selection Rules, Relaxation in Selection Rules. Nature of Electronic Spectral Bands: Band Widths, Band Intensities. Factors Influencing Band Shapes: Jahn-Teller Effect, Spectrochemical Series, Nephelauxetic Effect. Orgel Diagrams for d^1-d^9 Configurations, Crystal Field Spectra of O_h and T_d Metal Complexes of 3d Metals – Calculation of 10Dq Values, Racah Parameter (B) and Nephelauxetic Ratio (β) – Charge Transfer Spectra.

AC – 10 : IR & Raman spectroscopy

IR Spectroscopy: Principle, Instrumentation, sample handling, Fourier transform infrared spectroscopy- Principle, instrumentation & its advantages. IR in quantitative analysis. Applications of IR spectroscopy: structure analysis of organic compounds, inorganic molecules-Sulphato, Carbonato, Nitrato & metal chelates - Acetylacetanato Complexes. Analysis of petroleum hydrocarbons, oil and grease contents by EPA method, Quantitative analysis of multi-component mixtures.

Raman Spectroscopy: Theory, Instrumentation, sample handling and illumination, diagnosis, structure analysis, polarization measurements, quantitative analysis, laser applications,Resonance Raman spectroscopy and its applications.

AC – 11 Optical Methods 15 Hrs

Refractometry: Theory, instrumentation, specific and molecular refraction, Abbe, Pulfrich and immersiton types, applications

Polarimetry: Theoritical considerations – Plane polarized light, optical activity, specific and molecular rotations. Iinstrumentation,, applications.

Optical rotator dispersion and Circular dichorism: Optical rotation, circular birefringence, circular dichroism and Cotton effect, Octet Rule, Experimental Techniques, Applications : quantitative analysis,determination of absolute configuration, conformational studies and equilibrium studies. Use of CD in the conformational studies of metal complexes, DNA and DNA-metal complexes.

AC –12: Fluorimetry, Phosphorimetry, Nephelometry and Turbidimetry 15 Hrs

Fluorimetry and Phosphorimetry: Theory of Fluorescence and Phosphorescence- Excited states producing Fluorescence and Phosphorescence. Rates of absorption and emission. Deactivation processes, Variables affecting Fluorescence and Phosphorescence. Types of Photoluminescence spectra for Phenanthrene. Instrumentation – Components of Fluorimeter, Spectroflourimeters and Phosphorimeters. Applications of Fluorimetry- Determination of Inorganic Cations, Fluorimetric reagents. Fluorimetric determination of organic species – Thiamine, Aneurine Hydrochloride, Plolycyclic aromatic hydrocarbons. Phosphorimetry- Determination of Aspirin in blood serum. Chemiluminescence- Origin, measurements.

Analytical applications- Atmospheric pollutants (Oxides of Nitrogen and Sulphur compounds, Ozone). Detection in Gas Chromatography, High Performance Liquid Chromatography and Capillary Electrophoresis. Detection of Enzyme reaction products. Immunoassay and Nucleic acid assays.

Nephelometry and Turbidimetry: Principles and instrumentation for Nephelometry and Turbidimetry, Applications

Suggested Books

1. Principles of Instrumental Analysis– Skoog, Holler, Nieman, 5th ed., Harcourt College Publishers, 1998.
2. Introduction to Ligand Fields – Figgis, Wiley Eastern Ltd, 1966.
3. Inorganic Electronic Spectroscopy – A.B.P. Lever, Elsevier Publishing Company, London, 1968.
4. Chemical Analysis – A. K. Srivatsava & Jain, 3rd ed., S,Chand & Company Ltd., 1977.
5. Hand Book for Instrumental Techniques for Analytical Chemistry, Ed. Frank Settle. Prentice hall, New Jersey, USA, 1997.
6. Analytical Chemistry – Gary D. Christian, 6th ed, John Wiley and sons. Inc., New York, 1994.
7. Introduction to Inductively Coupled Plasma Emission Spectroscopy - GL Moore, Elsevier Science publishers, New York, 1989.
8. Analytical Chemistry – Skoog & West, 6th ed, W.B. Saunders, 1998.
9. Infrared and Raman Spectra of Inorganic and Coordination Compounds, Kazuo Nakamoto, 5th ed., John Wiley & Sons, 1995.
10. Vogel's Text book of Quantitative Analysis – J. Mendham et al, 6th ed., Pearson Education Ltd, 2002.
11. Instrumental methods of Analysis - Willard, 6th ed., CBS Publishers & distributors, 1986.
12. Analytical Chemisstry Instrumental techniques, Maninder Singh, Dominent Publishers, New Delhi, 2002.

Paper-IV

CH (AC) 304T: Separation Methods

AC-13 Solvent extractions

AC –14 Chromatography

AC – 15 Mass spectrometry & Hyphenated techniques

AC – 16 Electrophoresis

AC-13 Solvent extractions 15 Hrs

The distribution coefficient, distribution ratio, relation between KD& D, the percent extracted.

Solvent extraction of metals – ion association complexes, metal chelates, effect of pH and reagent concentration, extraction process, separation efficiency of metal chelates, analytical separations – multiple counter current distribution, solid phase extraction, solvent extraction of flow injection analysis. Super critical fluid extraction.

Organic reagents in Inorganic analysis - Theoretical basis for the use of organic reagents in inorganic analysis. Extraction of metal ions by the use of organic reagents – acetylacetone, thionyl-trifluoroacetone, tri-n-octyl phosphine oxide. Applications to extractions of metal ions by chelating agent (Dithiazone, 8-hydroxy quinoline and cupferron) Determination of salts of organic acids and bases, detemination of alkaloids in crude drugs.

AC –14 Chromatography 15 Hrs

HPTLC: Principle, Technique, advantages over TLC

Gas Chromatography (GC) – Theory, Data acquisition and processing Applications - Derivatization techniques. Monitoring of ethylene dibrombide (EDB) residue in Indian Black pepper by GC using electron capture detector. Analysis of petroleum products. Headspace analysis of tobacco. Preparative gas chromatography

High Performance Liquid Chromatography (HPLC) – Theory, and separation modes, Applications with respect to separation of enantiomers, Organic and inorganic systems.

Supercritical fluid chromatography (SFC) – Instrumentation of SFC, stationary and mobile phases used in SFC, Detectors, Advantages of SFC. Technique and applications of SFC.

Size Exclusion Chromatagraphy: Principle of Gel Chromatography, Filtration Chromatography, Instrumentation, retention behaviour, resolution, selection of gel type – applications . Ion Exclusion – Principle and applications.

Ultra Performance Liquid Chromatography: Principle, Instrumentation

AC-15 Mass Spectrometry & Hyphenated techniques 15 Hrs

Advanced Mass spectrometry

Quadruple analysers, Ion traps. Time of flight mass spectrometry.

Mass Spectrometry / Mass Spectrometry Tandem Mass Spectrometry. Ion cyclotron resonance spectrometers and Ion traps for MS/MS.

Quantitative mass spectrometry: Introduction, principle, calibration and internal standards.

Hyphenated techniques:

GC-MS: Principle, instrumentation, Interfaces, Mass analyzer, Mass chromatogram, Applications. Analysis of metabolite of drug Imipramine

GC-FT-IR: Principle, Instrumentation and Applications

LC-MS: Principle,Instrumentation, Interfaces and Applications.

LC-MS-MS : Principle, Instrumentation, Interfaces and Applications.

ICP-MS: Instrumentation, principles, Quantitative analysis and applications.

AC-16: Electrophoresis

Introduction, Definition

Paper Electrohoresis: Principle, Experimental Requirements, Technique, Factors governing the migration of ions, Applications

Capillary Electrophoresis: Electro osmotic flow, migration in CE, instrumentation, control of separation, applications

Gel Electrophoresis: Principle, technique, applications

Immunoelectrophoresis: Principle, technique, applications

Suggested Books

1. Separation Methods - M. N. Sastri, 1st ed., Himalaya Publishers, 1991.
2. Principles of Instrumental Analysis – Skoog, Holler, Nieman, 5th ed., Harcourt College Publishers, 1998.
29
3. Analytical Chemistry - Gary D.Christian, 6th ed, John Wiley and sons. Inc., New York, sixth edition, 1994.
4. Mass spectrometry for Chemists and Biochemists, Robert A.W. Johnstone and Macolm. E. Rose, 2th ed Cambridge University Press 1996.
5. Structural methods in Inorganic chemistry - E.A.V. Ebsworth, et al ELBS Publications,1988

6. Introduction to analytical Gas Chromatography, Raymond PW Scott,2nd Ed. Marcel Dekker, Inc. New York,1988.
7. Techniques and practice of Chromatography, Raymond PW Scott, Marcel Dekker, Inc. New York,1995.
8. Liquid Chromatography-Mass Spectrometry Principles & Applications, WMA Neissen & JV Greef, Marcel Dekker, Inc. New York,1992.

LABORATORY COURSE

Paper CH (AC) 351P: Titrimetry, Solvent extraction,Chromatography and Water analysis.

1. Titrimetry:
    1. Determination of Ca^{2+}, Mg^{2+}, CO_3^{2-} & HCO_3^- in soil sample.
    2. Determination of Calcium in Vitamin-D and Calcium tablelts
    3. Determination of Fe & Ca in Cement
    4. Determination of Saponification value and Iodine value of an oil sample

II. Solvent extraction:

1. Determination of Pb using Dithiazone

III. Chromatography (Demonstration):

1. Separation of Co & Ni in Cellulose column
2. Separation of amino acids in a mixture by TLC using Ninhydrin
3. Separation of additives in Ink by GC.
4. Separation of synthetic corticosteroids in by HPLC.

IV. Water analysis:

1. Determination of residual Chlorine in water by Iodometry
2. Determination of Dissolved Oxygen.
3. Determination of COD.
4. Determination of BOD.
5. Determination of residual Chlorine in water by Iodometry

Paper CH (AC) 352P: Colorimetry, Spectrophotometry

I. COLORIMETRY:

1. Determination of blood sugar
2. Determination of blood cholesterol
3. Determination of Paracetamol
4. Determination of Ampicillin
5. Estimation of Ascorbic acid

II. SPECTROPHOTOMETRY:

1. Determination of Manganese in steel
2. Determination of Phosphorous in human serum
3. Determination of Creatinine in a sample
4. Determination of pKa of an organic Indicator (Methyl Orange)
5. Simultaneous determination of Cr and Mn in an admixture
6. Spectrophotometric Titration of Fe(II) with o-Phen
7. Determination of composition of Complex by Job's Method and Mole ratio Method of Cu(II)-EDTA complex

SUGGESTED BOOKS

1. Chemistry Experiments for Instrumental Methods, Donald T Sawyer William R.Hememan etal John Wiley & Sons 1984.
2. Analytical Chemistry by Gary D.Christian 6th Edition John Wiley&Sons Inc New York 1994.
3. A Text Book of Quantitative Inorganic Analysis by A.I. Vogel 3rEdition

Elbs Publication 1969.
4. Vogel's Text Book Of Quantitative Inorganic Analysis Jeffery etal 4th edition Elbs Publications 1988.
5. Vogel's Text Book of Quantitative Chemical Analysis, 6th edition. Pearson Education Ltd 2002.
33
6. Analytical Chemistry Thoery and Practice by R.M. Verma 3rd Edn.CBS Publishers & Distrbutors1994.
7. Comprehensive Experimental Chemistry by V.K. Ahluwalia etal New Age Publications 1997.
8. Laboratory hand Book of Instrumental Drug Analysis.by B.G. Nagavi 2nd edn. 1996
9. Practical Pharmaceutical Chemistry, A.H. Beckett and J.B. Stenlake 4thedn. CBS publishers, 2001
10. Separation methods, MN Sastri, 2nd edn, Himalaya Publishing House1996
11. Hand book of analysis and quality control for fruit and vegetable products. S. Ranganna, 2nd edn, Tata MCGraw-Hill Publishing Company, 2002.
12. Gas Chromatography, Rajbir Singh, 1st edn, Mittal Publications, 2002

M.Sc.CHEMISTRY(ANALYTICAL CHEMISTRY)
IV SEMESTER SYLLABUS
(For the batch admitted during the academic year 2011-2012 under the CBCS pattern)
[Under Restructured CBCS Scheme]

Paper-I
CH (AC) 401T: Miscellaneous Methods of Analysis

AC – 17 Surface Analysis Methods
AC – 18 Diffraction Methods, X-Ray Absorption and X-Ray Fluorescence
AC –19 Electroanalytical Methods
AC – 20 Micromeritics, Dissolution and disintegration

AC-17 Surface Analysis Methods 15 Hrs

Introduction, types of surface measurements.
Photon Probe Tecnhniques: X-Ray Photoelectron spectroscopy - Principle, Instrumentation, applications.
Electron Probe Techniques: Scanning electron microscopy (SEM) – Principle, Instrumentation, applications. Electron Probe X-ray analysis (EPXMA) - Principle, Instrumentation, applications. Auger electron spectroscopy (AES) - Principle, Instrumentation, applications.
Ion Probe Techniques: Rutherford backscattering spectrometry (RBS) - Principle, Instrumentation, applications. Secondary ion mass spectrometry (SIMS) – Fundamental aspects of sputtering, Principle, Instrumentation (static & dynamic), applications
Scanning probe microscopy Techniques: Scanning Tunneling Microscopy – Principle, Instrumentation, applications. Atomic Force Microscopy - Principle, Instrumentation, applications.

AC-18 : Diffraction Methods, X-Ray Absorption and X-Ray Fluorescence 15 Hrs

X – ray Diffraction : X –rays and their generation – choice of radiation ; Miller indices, Braggs equation, Experimental methods – Powder and single crystal methods, Indexing the reflections, Systematic absences, Electron density studies by X – rays – Platinum phthalocyanine complex, Silyl acetate, Tetraalkyl biphosphate ; Advantages and limitations of X – ray Diffraction.
Electron Diffraction by gases : Principles, Applications to Silyl monothioacetate and Germyl monothioacetate and $HgCl_2$ molecules, Advantages and Limitations
Neutron Diffraction: Principle, Application in Hydrogen bonding studies, Advantages and limitations.
X-ray absorption method: Principle, radiographic non-dispersive x-ray Absorptiometers
X-ray fluorescence method: Instrumentation, qualitative and quantitative applications of XRF– advantages and limitations.\

AC-19: Electro Analytical Methods 15 Hrs

pH-metry: Accuracy of direct potentiometer measurements. The Glass pH electrode – Theory, construction, standard buffers, accuracy of pH measurements, measurements with the pH – meter, pH titration of unknown soda ash.
Electrogravimetry: Basic principles of electrogravimetry, Instrumentation, electrogravimetry determination with constant applied voltage and at constant current.

Applications of electrogravimetry. Problems based on effect of concentration on electrode potentials, calculation of theoretical cathode potential at the start of deposition, effect of pH in electrolytic separations.

Coulometry : Basic principles, Types of coulometers, constant current coulometric analysis, coulometric titrations – principle, circuit and cell for coulometry, Application to neutralization, Redox, precipitation, complexometric titrations, Advantages of coulometric titrations and errors. Controlled potential coulometry – Technique & applications of inorganic & organic compounds.

High Frequency Titrations

Introduction, Theory, Instrumentation, Applications, Advantages and disadvantages

AC-20: Micromeritics, Dissolution and disintegration 15 Hrs

Particle size analysis- concepts of particle size, size distribution, mean size of particulate system, methods of particle size analysis (sieving, microscopic method, sedimentation methods, electrical sensing zone method, optical sensing zone and light diffraction method). Dissolution: Drug absorption, theories of drug dissolution – Diffusion layer model, Danckwert's model & interfacial barrier model. Dissolution tests for tablets and capsules (basket apparatus, paddle apparatus, flow through cell apparatus). Disintegration tests for tablets, capsules and enteric coated tablets.

Suggested Books

1. Structural methods in Inorganic Chemistry - E.A.V. Ebsworth, et al., ELBS Publications, 1988.
2. Physical Methods in Chemistry - R.S. Drago, W.B. Saunders Co, 1977.
3. Instrumental Methods & Chemical Analysis – Galen Ewing, 5th ed., McGraw-Hill Publishing Company Ltd., 1985.
4. Analytical Chemistry - Gary D. Christian, 6th ed. John Wiley and sons. Inc, New York, 1994.
5. Principles of Instrumental Analysis – Skoog, Holler, Nieman, 5th ed., Harcourt College Publishers, 1998
6. Principles and practice of Analytical Chemistry, F.W.Fifield & D Kealey, 5th Ed. Blackwell Science, 2000.
7. Quantitative Chemical Analysis, Daniel C. Harris, 6th Ed. WH Freeman & Co. NewYork, 2003.

Paper –II

CH(AC) 402T:Applied Aalysis

AC –21 Industrial Analysis
AC –22 Analysis of Air and Water Pollutants
AC – 23 Clinical and Pharmaceutical analysis
AC – 24 Food and Agricultural analysis

AC –21 Industrial Analysis 15 Hrs

Analysis of Ferroalloys: Analysis of steel - Molybdenum, Phosphorous. Analysis of Ferromanganese, Ferrovanadium. **Analysis of non- Ferrous alloys**: Analysis of Tin, Zinc and Copper in Brass, Bronze. Analysis of Tin and lead in Solder. **Analysis of Cement**: Composition of Portland cement, estimation of Aluminium oxide and Ferrous oxide. Determination of Alumina in Cement by Polarography. **Analysis of Oils & Fats:** Theory, Melting point of fats, Chemical Characteristics: Saponification value, Iodine value, Thiocyanogen value, ketone or perfume rancidity. Analysis of fatty acid composition in oil by GLC, Oxidation levels of fats by TLC. **Soaps & Detergents:** Composition of Soaps. Determination of low level Surfactants, determination of Germicides in soaps and detergents by photometric method, analysis of phosphates by paper chromatography, determination of detergent alkylates by Mass Spectrometry. **Paints& Pigments**: Constituents of Paints, Analysis of Tio_2 in Titanium dioxide pigments by XRD. Determination of Zn, Pb in Paint pigments by Polarographic method. Analysis of polyesters, acrylics by Gel permeation chromatography.

AC-22 : Analysis of Air and Water Pollutants 15 Hrs

Analysis of Air Pollutants: Air quality standards, sampling, analysis of air pollutants-SO_2 (UV_Vis, IR), H_2S (Spectrophotometry and Non-dispersive IR Spectrophotometry), NO-NOx (Chemiluminescence technique, Colorimetric technique- Saltzman method), CO & CO_2 (IR, AAS & GC), Hydrocarbons (GC, GC-MS), Aromatic hydrocarbons in automobile exhaust, petrol, air, O_3 (Chemiluminiscence & Spectrophotometry), particulate matter analysis.

Analysis of Water Pollutants: Objectives of analysis, sampling, preservation and pre-concentration methods, physical analysis - colour, odour, temperature, pH, EC, redox potential, total desolved solids (turbidimetry), Chemical analysis of anions – CN-, Cl-, F-, NO_2-, NO_3- (spectrophotometry), SO_4, PO_4. Determination of BOD,COD, TOC & DO
Analysis of Toxic Metals: Hg, As, Pb, Cd, Be, Al, Cr (Atomic Absorption Spectroscopy and Spectrophotometry)

AC-23 : Clinical and Pharmaceutical Analysis 15 Hrs

Clinical Analysis: Determination of (1)Serum Calcium (2) Serum/Plasma Bicarbonate (Titrimetry).Determination of Serum Chloride (Coulometry) -Determination of (1) Cholesterol (2) Total Protein (3) Blood Urea in Serum (4) Amylase (5) Aspartate Amino Transferase (AST) and Alanine Amino Transferase (ALT) (by Spectrophotometry). Determination of (1) Thyroxin and (2) Thyroid-Stimulating Hormone (TSH) (by RIA Method)

Pharmaceutical analysis: Determination of Diclofenac (non-aqueous titration), Calcium in Vitamin D and Calcium formulations (Complexometry), Sulphanilamide (potentiometry), Pethidine hydrochloride (UV-Vis), Frusemide (UV-Vis), Aspirin, paracetamol and codein in APC tablets (NMR), Phenobarbitone in tablets (IR), pivolic acid in dipivefrin eye drops

(GC), Assay of hydrocortisone cream. (HPLC). Impurity profiling of Propranolol (GC-MS), famotidine (LC_MS).

AC -24: Food and Agricultural Analysis 15 Hrs

Food Analysis: Analysis of Chemical Additives in foods : Division of colour additives, Chromatographic identification of colours, and quantitative estimation of added dyes in foods (Titanium Trichloride Method) - chemical preservatives and synthetic sweetening agents (Organic-ether extractable and Non-ether extractable) - Analysis of SO_2 & Sodium Benzoate (Chemical Methods), Sorbic Acid (Chromatography) - Types of Antioxidants used in Foods, Analysis of Butylated Hydroxy Toluene (BHT) (Spectrophotometry).

Agricultural Analysis: Analysis of soils for available Major Nutrients - Estimation of available Nitrogen (Kjeldahl Method), Phosphorus (Olsen's Method and Bray and Kurtz Method), and Exchangeable Calcium & Magnesium (by EDTA). Soil analysis for Micronutrients - Estimation of Available Zinc, Copper, Manganese and Iron (AAS) - Analysis of Pesticide Residues - Determination of Methyl Parathion Residues in food grains & vegetables (Solvent Extraction and Titrimetry) - Determination of Organochlorine pesticides by Gas Chromatography (Cypermethrin) - Determination of Malathion and DDT Residues in food grains (Spectrophotometry).

SUGGESTED BOOKS

1. Analytical Chemistry, Gary Christian, VI Ed, John Wiley & Sons Inc, New York
2. Fundamentals of Analytcal Chemistry, Skoog & West
3. Pharmaceutical Drug Analysis, Ashtoshkar
4. Vogel's Text Book of Quantitative Chemical Analysis, 6th Ed, Pearson Education Ltd
5. Environmental Pollution Analysis, S M Khopkar, Wiley Eastern Ltd 1995
6. Environmental Analytical Chemistry, F W Fifield, P J Haines, Blackie Academic& Professional.
7. Environmental Chemistry, B K Sharma, Goel Publishing House, Meerut.
8. Handbook of Analysis and quality control for fruit and vegetable products, S Ranganna, Tata Mc Graw Hill Publishers Ltd, 1986
9. Introduction to chemical analysis of foods, S Suzanna & Nielsen, CBS Publishers & Distributors
10. Practical pharmaceutical Chemistry, a H Beckett and J B Stenlake, III Ed, Vol I and Vol II, CBS Publishers & Distributors,1997
11. Pharmaceutical Analysis, David G Watson,Churchill Livingstone Harcourt Brace and Company Ltd, 1999
12. Handbook of analysis of drugs, Nagavi
13. Medical Laboratory Technology – Mukherjee , Tata Mc Graw Ltd 1988.
14. Medical Laboratory Technology – Ramnik Sood , Jaypee Brothers Ltd 1999.
15. Text Book of Clinical Chemistry V Edn Carl.A. Burtis Edward R. Ashwood Saunders Harcourt India 2001.

Paper-III

CH (AC) 403T: Laboratory Management

AC – 25 Automation in laboratory
AC – 26 LIMS & Computer aided analysis
AC – 27 Laboratory Management & Standard reference materials
AC – 28 Accreditation of Laboratories, Quality management

AC- 25 Automation in Laboratory. 15 Hrs

Introduction, classification of Analytical methods, Types of Instrumental methods, Instruments for analysis. Analog & Digital signals, Planning for laboratory automation. An overview of automatic instruments & instrumentation.
Flow Injection Analysis, Discrete Automatic systems.
Good laboratory practices: Instrumental standardization, optimization of procedures.

AC-26 LIMS and Computer aided Analysis 15 Hrs

Laboratory Information Management System: Laboratories as information producers, properties of good information, Laboratory information management system, conclusions.
Computer aided analysis: Computer-instrument interaction, computer organization-Hardware - Basic Digital circuit components, Microprocessors and Microcomputers, Computer Software - Software control of the computer-instrument interfaces. Automated laboratory – Automated instruments (AAS), Applications of computers, Computer Networks.

AC- 27 Laboratory Management & Standard reference materials 15 Hrs

Introduction – Administration, Geographical location of the laboratory, relationship with the industrial exploratory and regulatory work and the analytical laboratory. Disciplines represented in the Laboratory. Educational requirements of the laboratory personnel. Work load statistics of the laboratory coordination between routine work and research cell. Regular academic research work, opportunities for training. Internal organization of the laboratory. Architectural issues, laboratory infrastructure of equipment and instrumentation.

Standard reference materials

Standards of Analysis, Analytical standards, reference materials, High purity substances, working and secondary standards.

AC- 28 Accreditation of Laboratories, Quality Management 15 hrs

Accreditation of Laboratories: International organization for standardization, National accreditation board for testing and calibration laboratories. Scope of accreditation.
Analytical Methods: choosing the methods- standard methods, official methods, literature methods. Validation of new methods - comparison of analytical methods.
Quality systems, the operational aspects required to deliver a quality system (Traceability, quality control, quality assurance, quality management and quality manual) calibration and test methods.
Total Quality Management (TQM) – Essentials of TQM: Quality Planning, Quality control, Quality Audit, Quality surveillance, Quality assurance, Quality circles.
Analytical methods of validation:Characteristics of Analytical procedures – Accuracy, precision, linearity, Range specificity,Detection limit, Quantitation limit, robustness process validation, Types of process validation –prospective, concurrent and retrospective process validation.

Suggested Books

1. Principles of Instrumental Analysis - Skoog. Holler, Nieman, 5th ed., Harcourt College Publishers, 1998.
2. Model for Quality assurance in design/development production, installation and servicing, ISO 9001.
3. Journal of Validation technology, Vol.-III and IV, 1997.
4. Instrumental Methods of Analysis - Willard, Merit, Dean, 6th ed., CBS Publishers & distributors, 1986.
5. Hand Book for Instrumental Techniques for Analytical Chemistry, Ed. Frank Settle, Prentice Hall, New Jersey, USA, 1997.
6. Handbook of Quality Assurance for the analytical chemistry laboratory, James P. Dux, Van Nostrand Reinhold, New York, 1986.
7. Quality in Totality – Parag Diwan, Deep & Deep Publications, 1st ed., 2000.
8. QA manual – DH Shah, Business Horizons, 1st ed., 2000.

PAPER – IV: CHOICE BASED PAPER -1

CH (AC)(CB_1) 404T : Quality Assurance and Accreditation

AC(CB_1) -1 Quality Assurance – I
AC(CB_1) -2 Quality Assurance – II
AC(CB_1) -3 Quality Assurance – III
AC(CB_1)- 4 Quality Accreditation

AC(CB_1) -1: Quality Assurance – I 15 Hrs

Introduction to Quality Control and quality assurance: Concepts and significance.

Quality control and statistical techniques: Quality control charts, the X-quality control chart, the R-quality control chart and its interpretation, spiked sample control charts, use of blind samples in quality control, use of proficiency evaluations in quality control.

Calibration and maintenance of Instruments / Equipment: Instrument calibration – linear calibration curves, equipment calibration, frequency of calibration, calibration of common laboratory instrument and equipment (Analytical balances, volumetric glassware, ovens, furnaces, UV / Visible spectrophotometer, pH meter, conductivity meter, IR spectrophotometers, AAS, GC, HPLC etc.,). Maintenance of instruments and equipment.

AC(CB_1) 2: Quality Assurance – II 15 Hrs

Documentation for quality assurance: Raw Data - Type of notebooks, control of notebook distribution and data entry. General Reagents and volumetric reagents. Sampling – sampling methods, sample labeling, sample log-in/register. Sample analysis, reporting, recording and personal training. Instrument calibration and maintenance. Analytical report. Personnel, training, records - professional personnel, technician personnel. Filing quality assurance documentation.

Good laboratory practices and personnel, Quality Programme, Instrument and **:** Organisation calibration, Customer Satisfaction.

AC(CB_1) -3: Quality Assurance – III 15 Hrs

Computers and quality assurance: Sample handling. Data Acquisition. Quality control data and calculations. Computer generated analytical reports. Security considerations. Hardware and software.

Establishing a Quality Assurance program: Management commitment. Define the quality assurance program. Writing standard operating procedures. Topics for standard operating procedures. Consolidating the programme. Monitoring the program – monitoring quality assurance data, reporting quality assurance problems. Writing the quality assurance manuals.

AC(CB1) -4: Quality Accreditation: 15 Hrs

Laboratory Accreditation: Need for laboratory accreditation. International aspects of laboratory accreditation and in India. Criteria for laboratory accreditation. Benefits of laboratory accreditation,

Evolution and significance of Quality Management, Background to ISO 9000, comparison between ISO-9001, ISO-9002 & ISO-9003., ISO 9000-2000 series of standards on quality managament system, - evolution of series of standards, introduction to ISO organization, Registration / certification - benefits of QMS certification. Structure of ISO 9000-2000 family of standards. Advantages of ISO 9000-2000. Requirements of ISO 9001-2000 QMS and applications, Steps for effective implementations. Significance of ISO - 9001,9002,9003 & 9004.

Requirements of ISO9000/IS14001. Concepts of OHSMS (BS 8800) Quality Managament Principles in QMS, QMS documentation, Quality Manual, Quality policy, conformities and Non-confirmities.

Suggested Books:

1. Handbook of Quality Assurance for the analytical chemistry laboratory, James P. Dux, Van
Nostrand Reinhold, New York, 1986.
2. Applying ISO-9000 Quality Management Systems, International Trade Centre Publishing, UNCTAD/WTO. Geneva, Switzerland, Indian Edition Printed by D.L.Shah Trust.
3. How to practice GLP, PP Sharma, Vandana Publications, 2000, New Delhi
4. Training manuals on ISO 9000 / 2000 PQM, Girdhar J Gyani, Raj Publishing House, 2001
5. Quality Assurance in Analytical Chemistry, B.W. Wenclawiak, Springer,India, 2004.

PAPER – IV: CHOICE BASED PAPER -2

CH (AC)(CB_2) 404T : Applied analysis and Green Analytical Chemistry

AC(CB_2) -1 Enzyme catalysis- Analytical applications
AC(CB_2) -2 Forensic Chemical Analysis
AC(CB_2) -3 Limit tests
AC(CB_2)- 4 Green Analytical Chemistry

AC(CB_2) -1 Enzyme catalysis- Analytical applications 15 Hrs

Basic principles, Catalysis – measurement of catalytic reactions, Nonspecificity of catalysts, types of reactions catalyzed. Enzyme catalysis, enzyme kinetics, properties of enzymes, enzyme inhibitors and activators, enzyme specificity, Determination of enzymes and enzyme substrates. Example of enzymatic analysis: Dehydrogenase reactions, Substrate determinations: Glucose, Uric acid. Immobilized enzymes. Evaluation methods.

AC(CB_2) -2 Forensic Chemical Analysis: 15 Hrs

Contact traces – Analysis of soil, fiber and paint evidence in forensic work.

Analysis of narcotic drugs and psychotropic substances (opiates, cannabinoids, barbiturates, benzodiazepines, amphetamimes with one example each and LSD) by colour/micro crystal tests, chromatographic methods (TLC, GC, and LC) and spectroscopic methods (UV-Vis, IR, MS and GC-MS). Analysis of explosives and explosion residues(Low explosive residues – cations and anions; High explosive residues – RDX) by spot tests, chromatographic methods (TLC, GC AND GCMS) and spectroscopic methods (UV-Vis, IR, MS and GC-MS).

Analytical toxicology – extraction techniques for dugs and pesticides – analytical techniques in forensic toxicology for alcohols, drugs and pesticides involving spot tests (TLC, GC & LCMS). Interpretation of analytical data – court testimony.

AC(CB_2) -3 Limit tests 15 Hrs

Limit tests for insoluble matter, limit tests of soluble matter, limits of moisture, volatile matter, residual matter, residual solvents, limits of nonvolatile matter, limits of residue on ignition, limits of loss on ignition, limits on ash value. Limit tests for metallic impurities: lead, arsenic, iron: Limit tests for acid radical impurities, chlorides, sulfates, arsenate, carbonate, cyanide, oxalate, phosphate. Limit tests for nonmetallic impurities: Boron, free Halogens, Selenium.

AC(CB_2)- 4 Green Analytical Chemistry 15 Hrs

Green Analytical Chemistry: Concepts and trends

"Greening" Sample Treatment: Reduced and solvent- free sample preparation methodologies, alternative solvents, energy saving procedures.

Green Instrumental Analysis: Assessment of analytical methods for "Greenness", greening flow injection analysis, chemical sensors, liquid green chromatography.

Suggested Books

1.Analytical Chemistry - Gary D. Christian, 6th ed. John Wiley and sons. Inc, New York,1994.

2. Kinetics methods of analysis – Marck & Rekniz Vol25

3. Practical Pharmaceutical Chemistry, A.H. Beckett et al, 3rd ed. – Vol. 1 & Vol. 2 CBS Publishers & distributors, 1986.

4. Green Analytical Chemistry: Theory & Practice, Miguel De La Guardia, Sergio Armenta, Elsevier

5.Green Analytical Chemistry, Mihkel Koel, Mihkel Kaljurand, RSC Publishing

LABORATORY COURSE

Paper CH (AC) 451P: Electro analytical techniques:

I. POTENTIOMETRY:

1.Determination of Ferrous using $K_2Cr_2O_7$

2.Determination of iron in iron wire using $KMnO_4$

3. Determination of a mixture of Ferrous and Vanadyl using Ceric ammonium nitrate

4. Determination of silver in silver metal

5. Assay of sulphanilamide in samples

Use of ion selective electrodes:

6.Determination of mixture of halides using Ag ion electrode

II. pH METRY:

1. Strong acid Vs strong base titration

2. Mixture of acids Vs strong base

3.Determination of mixture of carbonates and bicarbonates

4. Determination of Dissociation constants of Histidine monohydrochloride

5. Determination of binary stability constants of Cu(II) – Histidine complexes

III.POLAROGRAPHY:

1. Polarographic determination of Cu & Zn in brass

IV. CONDUCTOMETRY:

1. Mixture of acids Vs strong base titration

2. Mixture of bases Vs strong acid titration

3. K_2SO_4 Vs $BaCl_2$ titration.

4.Determination of the composition of Cu(II) oxine complex

5. Determination of Quinine dihydrochloride with NaOH

6. Determination of Aspirin with KOH

Paper CH (AC) 452P: Spectroscopic Techniques , Spectral problems and Evaluation of Physical Parameters Of Tablets

I. FLAME PHOTOMETRY:

1. Determination of i)Na, ii)K, iii)Ca, iv)Li

II. FLUORIMETRY

1. Determination of Vitamin – B_1 (Thiamine)

2. Determination of Vitamin – B_2 (Riboflavin)

3 . Determination of Quinine sulphate.

III. ATOMIC ABSOPTION SPECTROSCOPY

1.Determination of i) Fe, ii) Zn, iii) Cu, iv) Pb.

IV. Structural elucidation based on spectral data from UV – Vis, IR, NMR and Mass Spectrometry

V. EVALUATION OF SOME PHYSICAL PARAMETERS OF TABLETS:

1. Dissolution profile of Ampicillin.

2. Disintigration test for Ibuprofen (coated tablet).

3. Determination of friability of Paracetamol tablet.

SUGGESTED BOOKS

1. Chemistry Experiments for Instrumental Methods, Donald T Sawyer William R.Hememan etal John Wiley & Sons 1984.
2. Analytical Chemistry by Gary D.Christian 6th Edition John Wiley&Sons Inc New York 1994.
3. A Text Book of Quantitative Inorganic Analysis by A.I. Vogel 3rEdition Elbs Publication 1969.
4. Vogel's Text Book Of Quantitative Inorganic Analysis Jeffery etal 4th edition Elbs Publications 1988.
5. Vogel's Text Book of Quantitative Chemical Analysis, 6th edition. Pearson Education Ltd 2002.
6. Analytical Chemistry Thoery and Practice by R.M. Verma 3rd Edn.CBS Publishers & Distrbutors1994.
7. Comprehensive Experimental Chemistry by V.K. Ahluwalia etal New Age Publications 1997.
8. Laboratory hand Book of Instrumental Drug Analysis by B.G. Nagavi 2nd edn. 1996
9. A Text Book of Quantitative Inorganic Analysis by A.I.Vogel 3rd Edition, ELBS Publication 1969.
10. Determination and use of Stability Constants – Martell and Motekaitis VCH Publishers INC 1988.
11. Metal Complexes in Aqueous Solutions A.E.Martell and R.D. Handcock, Plenum Press, New York – 1996.
12. Experiments in Chemistry, D.V. Jahagirdar, 2nd edn, Himalaya Publishing House, 2003
13. Practical Pharmaceutical Chemistry, A.H. Beckett and J.B. Stenlake 4thedn. CBS publishers, 2001

DEPARTMENT OF CHEMISTRY ,OSMANIA UNIVERSTY
M.Sc.Chemistry.
Five Year Integrated Course
(Offered at Department of Chemistry,NizamCollege,Basheerbagh,Osmania University)
IX&X Semester
(effective from academic year 2012-2013
Approved in BOS Chemistry (PG)

Semester IX

THEORY

	Hrs/week	Internal assessment	Semester exam	Total
FYIC-901T	4	20 marks	80 marks	100 marks
FYIC-902T(E)	4	20 marks	80 marks	100 marks

PROJECT

	Hrs/week	Pre-Viva	Seminar	Project Evaluation	Total
FYIC-Proj,I					
Project	26	100	40	260	400 marks
Seminar	2				
Total	**34+2**				**600 marks**

Note : E-Elective Paper

Semester X

THEORY

	Hrs/week	Internal assessment	Semester exam	Total
FYIC-1001T	4	20 marks	80 marks	100 marks
FYIC-1002T(E)	4	20 marks	80 marks	100 marks

PROJECT

Hrs/week	Pre-Viva	Seminar	Project Evaluation	Total
FYIC-Proj,II				
Project 26	100	40	260	400 marks
Seminar 2				
Total 34+2				**600 marks**

Note : E-Elective Paper

Five Year Integrated M.Sc. Course
SEMESTER IX

Paper I 901
Research, Methodology and Manuscript Writing

Technical Writing
Specific kinds of technical writing
Report Writing
Various kinds of reports

Paper II
Elective I: 902

902(E1): Organo metallic Chemistry of Transition Metal Complexes.

OMC-01 Mono,Di,Tri and Tetra hapto Complexes
OMC-02: Penta,Hexa,Hepta and Octa hapto Complexes
OMC-03: Catalytic Role of OTMC-I
OMC-04: Catalytic Role of OTMC-II

902(E2): Bioorganic Chemistry

BO-01: Enzymes and their action
BO-02: Enzyme models and Enzymatic transformations
BO-03: Recombinant DNA and Fermentation technology
BO-04: Coenzymes

902(E3): Catalysis

CS-01: Homogeneous catalysis
CS-02: Surface Chemistry & Micellar catalysis
CS-03: Heterogeneous catalysis
CS-04: Phase transfer , Anchored & Photo catalysis

Five Year Integrated M.Sc. Course
SEMESTER IX

Paper I 901
Research, Methodology and Manuscript Writing

UNIT I
Technical Writing:

Introduction
Organization and language
The writing process (pre-writing, writing, rewriting)

UNIT II
Specific kinds of technical writing:

Writing definitions
Précis writing
Abstract writing
Technical descriptions
Process description
Proposal writing

UNIT III
Report Writing:

Theory and practice
Routine and special reports
Methods of reporting (letter method and schematic method)

UNIT IV
Various kinds of reports:

General structure
Lab reports
Project report
Survey report
Feasibility

Recommended Reading:

1. **"Communication Skills"** by Joy Anuradha et al, published by Pearson, 2012, Delhi, India.

2. **"Communication Skills for Engineers"** 2nd Edition, by C. Muralikrishna and Sunita Mishra, Published by Pearson Education, 2011, Delhi, India.

3. **"Effective technical Communication"** by Ashraf Rizvi, published by Tata McGraw – Hill Publication Company, New Delhi, 2005.

Paper II

Elective I: 902

902(E1): Organo metallic Chemistry of Transition Metal Complexes.
902(E2): Bioorganic Chemistry
902(E3): Catalysis

E1: Organo metallic Chemistry of Transition Metal Complexes

OMC-01 Mono,Di,Tri and Tetra hapto Complexes
OMC-02: Penta,Hexa,Hepta and Octa hapto Complexes
OMC-03: Catalytic Role of OTMC-I
OMC-04: Catalytic Role of OTMC-II

OMC-01: Mono,Di,Tri and Tetra hapto Complexes

Nomenclature and Classification based on the number of Coordinated Carbons (hapticity) and number of electrons donated by the Ligand. η1 – Complexes : General methods of Preparation – Bonding of Ligand to Metal :α and β Interaction – Thermodynamic Stability and Kinetic Lability of η1 Complexes –Tertiary Phosphine – Transition Metal Alkyl and Aryl Complexes of Ni, Pd and Pt – Ortho-effect – Bonding in Metal – Carbene and Carbyne Complexes. η2 – Complexes : General methods of preparation of Metal – Alkene Complexes – Structure and Bonding in η2 Complexes – Factors affecting the stability of Metal-Olefin bond – Trans Effect – Rotation of Olefin around Metal-Olefin Bond. η3 - Complexes : Metal-Allyl Complexes – General Preparative Routes – Structure and Bonding in η3 Allyl Complexes – Fluxionality – Reactions of η3 Allyl Complexes. η4 Complexes : Structure and Bonding in η4 Complexes – Butadiene and Cyclobutadiene Complexes and their Reactivity.

OMC-02: Penta,Hexa,Hepta and Octa hapto Complexes

η5 – Complexes : Classification and General methods of Preparation – Bis (η5-cyclopentadienyl) metal complexes (Metallocenes) – Ferrocene : Structure and Bonding –Reactions of Ferrocene – Mechanism of Electroplilic substitution – Friedel Crafts acylation, alkylation, nitration, halogenation and Metallation Reactions.
η6 Complexes : Metal –Arene Complexes – Dibenzenechromium – Preparation, Structure and Bonding in Bis(arene)-Metal Complexes – Reactions. η7 Complexes : Preparation , Structure and Reactions of η7 – C_7H_7 Complexes. η8 Complexes : C_8H_8 as a Ligand – Cyclooctatetraene Complexes – Preparation, Structure and Bonding in Uranocene.

OMC-03: Catalytic Role of OTMC-I

Oxidative addition and Reductive Elimination : Stereochemistry and Mechanism of Oxidative Addition – Insertion Reactions – Hydrogenation of Olefins –Transfer Hydrogenation – Hydrosilation of Olefins – Isomerisation of Olefins – Ziegler –Natta Polymerization of Olefins – Oligomerization of Butadiene Alkene Metathesis.
Oxidation of Olefins to Carbonyl Compounds – Oxidation of Hydrocarbons to Alcohols and Acids – Oxidation of Aldehydes.

OMC-04: Catalytic Role of OTMC-II

Reactions of Carbon monoxide and Hydrogen : Hydroformylation – Carbonylation –Syngas-Water gas shift Reaction (WGS) – Reactions of Syngas. Applications of Metal Clusters in Catalysis : Hydroformylation of Ethylene using $[HRu_3(CO)_{11}]$ – , Hydrogenation of Olefins. Use of $[Fe_6C(CO)_{16}]$ as a model for Fischer – Tropsch process. Recent Developments in Homogenous Catalysis: Phase Transfer Catalysis (PTC) – Homogeneous Transition Metal Catalyzed Reactions under Phase Transfer Conditions : Hydrogenation. Bio Catalysis : Enzyme Analogue Catalysis : Introduction, Examples of Enzymatic Conversions, Reduction of >C=O and >C=C< bonds, Templates: Introduction, Metal Cations as Templates , Covalent molecules as Templates, External and Internal Templates – Homogeneous Catalysts and their Heterogenization or Immobilization by Aqueous Catalysis.

SUGGESTED BOOKS

1.*Organometallics*-A Concise Introduction, Ch.Eischeinbroich and Salzer-VCH
2.*Organotransition Metal Chemistry Fundamental Concepts and Applications*, John Akio Yamamato, Wiley & Sons.
3.Homogeneous Catalysis by Metal Complexes, M M Taqui Khan and A E Martel
4. Applied Homogenous Catalysis with Organo Metallic Compounds Vol I & II, Boy Cornills and W A Herrmann – VCH
5. Organometallic Compounds, G E Coates, M C H Green, K Wade vol II
6. Advanced Inorganic Chemistry, Cotton and Wilkinson, V & VI Ed
7. Symmetry and spectroscopy, K Veera Reddy
8.Homogenous catalysis, G W Parshall, John Wiley & Sons, New York

E2 : Bioorganic Chemistry

BO-01: Enzymes and their action
BO-02: Enzyme models and Enzymatic transformations
BO-03: Recombinant DNA and Fermentation technology
BO-04: Coenzymes

BO-01: Enzymes and their action **15 Hrs**

Introduction to enzymes. Transition state theory. Acid-Base catalysis. Covalent catalysis— Binding modes of catalysis (i) Proximity effect (ii) Transition state stabilization (iii) Strain and Distortion. Examples of some typical enzyme mechanisms for (1) Triose phosphate isomerase, (ii) α-chymotrypsin and serine protease (iii) Lysozyme (iv) Carboxy peptidase-A (v) Ribonuclease.

BO-02: Enzyme Models and Enzymatic transformations **15 Hrs**

Introduction — Biomimetic chemical approach to biological systems-Enzyme models Advantage of enzyme models. Requirements necessary for the design of enzyme models. Host-Guest complexation chemistry. Examples of some host molecules-Crown ether cryptanes, cyclodextrins. Cyclodextrin based enzyme models-Valixarenes, ionophores, micelles and synzymes (synthetic enzymes) — chiral recognition and catalysis.Introduction to industrial enzymes. Enzymatic synthesis of α-amino acids and peptides. Transformations of lipases and esterases. Kinetic resolutions of catboxylic acids, esters and alcohols - Transesterification. Amine resolution-use of oxido-reductase. C-C bond formation using enzymes-asymmetric cyanohydrin formation and asymmetric aldol condensations.

BO-03: Recombinant DNA and Fermentation technology **15 Hrs**

Introduction to genetic engineering. Recombinant DNA technology-restriction endonuclease, cloning, linkers, adaptors. Application of recombinant DNA technology in production of pharmaceuticals, diagnosis of diseases, insect control, improved biological detergents, gene therapy-examples. Principles of finger printing technology- Site directed mutagenesis. Fermentation technology: Introduction to fermentation. Industrial fermentation. Advantages and limitations of fermentation. Production of drugs and drug intermediates from fermentation-examples. Chiral hydroxy acids, vitamins, amino acids, β-lactam antibiotics. Precursor fermentation and microbial oxidation and reductions.

BO-04: Coenzymes **15 Hrs**

Introduction. Co factors — cosubstrates — prosthetic groups. Classification — Vitamin derived coenzymes and metabolite coenzymes.Structure and biological functions of coenzyme A, thiamine pyrophosphate (TPP), pyridoxal phosphate (PLP), oxidized and reduced forms of I) nicotinamide adenosine dinucleotide / their phosphates (NAD), NADH, $NADP^+$ NADPH) ii) Flavin adenine nucleotide FAD, $FADH_2$ and iii) Flavin mononucleotide (FMN, $FMNH_2$) lipoic acid, biotin, tetrahydrofolate and ubiquinone. Adenosine triphosphate (ATP) and adenosine diphosphate (ADP), S-adenosyl methionine (SAM) and uridine diphospho sugars (UDP-sugars) Mechanism of reactions catalysed by the above coenzymes

Recommended Books

I. Concepts in biotechnology by D. Balasubramananian & others
2. Principals of biochemistry by Horton & others.
3. Bioorganic chemistry - A chemical approach to enzyme action by Herman Dugas and Christopher Penney.
4.Chirotechnology by R.Sheldon

E3: Catalysis

CS-01: Homogeneous catalysis
CS-02: Surface Chemistry & Micellar catalysis
CS-03: Heterogeneous catalysis
CS-04: Phase transfer , Anchored & Photo catalysis

CS-01: Homogeneous catalysis. (15 hrs)

Introduction to catalysis. Types of catalysis, characteristics of catalyst, catalyst supports, promoters, general mechanism of catalysis, equilibrium treatment and steady state treatment. Activation energies of catalyzed reactions. Acid-base catalysis, general acid base catalysis, mechanism of acid –base catalysis, catalytic activity and acid-base strength- Bronsted relationships.

Acidity functions: The Hammett acidity function. Measurement of Hammett acidity function(Ho), usefulness of Hammett acidity function in understanding the mechanism of an acid catalyzed reactions. Zucker-Hammett hypothesis and the Bunnett's theory.

Catalysis by transition metal ions and their complexes. Use of Ziegler –Natta and metallocene catalysts as homogeneous catalysts for polymerization of olefins. Some industrially important catalytic processes. The Waker process, the hydrogenation of alkenes.

CS-02: Surface Chemistry & Micellar catalysis (15hrs)

Surface tension. Curved interfaces. The Laplace equation. Capillary action. Thermodynamics of surface layers – Gibbs isotherm.
Adsorption. Types of adsorption, factors effecting adsorption, determination of heats and entropies of adsorption. Surface versus bulk structures. Adsorbate -induced restructuring of surfaces. Thermal activation of bond breaking on a surface. Co-adsorption. Chemisorption isotherms. Kinetics of chemisorption. Surface films. Monometellic surfaces and bimetallic surfaces. Experimental techniques for the study of monolayer films. States and reaction in monomolecular films. Reaction between $H_2(g)$ and $N_2(g)$ catalyzed by surfaces to give $NH_3(g)$. Solid-liquid boundary- charged interface, electrokinetic phenomena. Streaming current, streaming potential, electro osmosis and electro osmotic pressure – electrical double layer and explanation of these phenomena. The zeta potential and its determination. Sedimentation potential.
Micelles: Classification of surface active agents .Micellization and micellar interactions, Structure of micelles – spherical and laminar**.** Critical micellar concentration (CMC). Factors affecting the CMC of surfactants. Counter ion binding to micelles. Thermodynamics of micellization. Phase separation and mass action models, solubilization, micro emulsion, reverse micelles reactions assisted by micelle formation. Examples of micelle-catalyzed reactions and their mechanisms.

CS-03: Heterogeneous catalysis. (15 hrs)

Heterogeneous catalysis. Broad categories of catalysts – metals, bimetals, semiconductors, insulators, zeolites, oxides, nano materials.

Preparation of metal catalysts , supported metal catalysts and non- metallic catalysts

Characterization of catalysts: Surface area by BET method. Determination of pore volume and pore size distribution by BJH method. Pore size and specificity of catalysts. Surface acidity of catalysts- Determination of surface acidity by indicator method , IR spectroscopic method and TPD methods. Surface characterization by XRD, LEED, STM & AFM, XPS, AES, LEIS techniques.

Steps in heterogeneous catalyzed reactions. Diffusion and adsorption. Mechanism of surface-catalyzed reactions. The Langmuir-Hinshelwood and the Eley-Rideal mechanism. Rate constants and activation energies of surface reactions. Catalytic activity – the determining factors. Cracking and reforming, auto exhaust emissions- catalytic converters. Catalytic hydrogenation and oxidation reactions. Cracking and reforming. Fischer-Tropsch synthesis of methanol. Structure sensitive and structure insensitive catalyats. Autoexhaust emissions-catalytic converters.

CS-04: Phase transfer, Anchored & Photo catalysis **(**15 hrs)

Phase-transfer catalysis (PTC): Principles of phase-transfer catalysis. PTC classification. Role of water in phase-transfer catalyzed reactions. Factors influencing the rate of PTC reactions. Inverse phase transfer catalysis. Mechanism of nucleophilic displacement reactions. Crown ethers. Crown ethers as PTCs in the reaction of alkyle halides with super oxide. Permanganate oxidation of alkenes and phenols in the presence of quarternary ammonium salts and crown ethers as PTCs

Anchored catalysis: Definition and examples of anchored catalysis- organic polymers, inorganic oxides and clays as supports. Structure of montmorillonite anchored catalysts- HEW structure and EF structure. Montmorillonite anchored catalysts- Application of intercalated clay catalysts-application of intercalated clay catalysts in hydrogenation reactions.

Photo catalysis: Photocatalytic effect, metal semiconductor systems as photo catalysts, nature of the metal loaded, extent of metal loading, nature of semiconductor, doped semiconductors, coupled Semiconductors. Application of photocatalysis for splitting of water by semiconductor particles, removal of organic and inorganic pollutants, for oxidation and reduction of organic compounds.

Books suggested:

1. Principles of Heterogeneous Catalysis in practice, G. C. Bond, Oxford Publishing
2. Heterogeneous Catalysis, C. Satterfield, McGraw Hill
3. Catalysis, Principles and applications, edited by B. Vishwanathan, S. Sivasanker & A. V. Rama Swamy, Narosa Publishing House
4. Catalysis, J. C. Kuriacose, Macmillan
5. Colloidal and surface chemistry , M. Satake, Y. Hayashi, Y.Mido, S.A.Iqbal and M.S.sethi
6. " Physical Organic Chemistry" by L.P.Hammett, chapter 9 , McGraw Hill .
7. Chemical Review, **57,** 1935(1957), M.A. Paul and F.A. Long
8. Phase Transfer Catalysis, Fundamentals, Applications and Industrial perspective, C. M. Stark, C. Liotta & M. Halpern, Academic Press
9. Phase Transfer Catalysis, E. V. Dehmlow & S. S. Dehmlow, Verlag Chemie, Weinheim
10. Phase Transfer Catalysis in Organic synthesis, W. P. Weber & G. W. Gokel, Springer
11. Hand book of phase transfer catalysisEdited by Y. Sasson and R. Neumann
12. Catalysis in Micellar and Macromolecular systems, J. H. Feudler & E. J. Feudler, Academic Press
13. Reaction Kinetics in Micelles, E. H. Codes (ed), Plenum
14. Micelles – Theoretical and Applied aspets, V.Moroi, plenum
15. Physical Chemistry of surfaces, A.W.Adamson and A.P.gast, Wiley

Polymer supported Catalysts, C. U. Pittman Jr, vol 8, Comprensive Organometallic Chemistry

Laboratory course
Project I

Five Year Integrated M.Sc. Course
SEMESTER X

Paper I: 1001
Intellectual Property rights

IPR - 01 : Introduction to IPR
IPR - 02 : International Organizations & Treaties
IPR - 03 : Patent Search
IPR - 04 : IP Reports Generation

Paper II
Elective II: 1002

1002(E1): Green Chemistry

GC- 01: Introduction to Green Chemistry
GC-02: Approaches to green synthesis
GC-03: Microwave Induced and ultrasound assisted green synthesis
GC-04: Organic synthesis in aqueous phase and in solid state

1002(E2): Pharmaceutical Analysis

PA 01: Spectral Methods in Pharmaceutical Analysis
PA 02: Chromatography in Pharmaceutical Analysis-I
PA 03: Chromatography in Pharmaceutical Analysis-II
PA 04: Titrimetry, Chemical and Extraction methods in Pharmaceutical Analysis

1002(E3): Pharmaceutical design, development and computer application

PD - 01 : Principles of Drug Discovery
PD - 02 : SAR Studies
PD - 03 : QSAR Studies and Structure Based Drug Design
PD - 04 : Computational Chemistry and Molecular Modelling

Five Year Integrated M.Sc. Course
SEMESTER X

Paper I: 1001
Intellectual Property rights

IPR - 01 : Introduction to IPR
IPR - 02 : International Organizations & Treaties
IPR - 03 : Patent Search
IPR - 04 : IP Reports Generation

IPR - 01: Introduction

Introduction : Legal Rights and obligations, Concept of Property, Kinds of Property, General concept and Significance of Intellectual Property (IP), Intellectual Property Rights (IPR), Intellectual property, Introduction to IPR, contents of IPR and their protection, Recent Developments, IP Organisations.
Introduction to Patents, Trademarks, Copyrights, Trade secrets, Industrial designs and Geographical indications.

IPR - 02: International Organizations & Treaties

Paris Convention for the Protection of Industrial Property, Berne Convention for the Protection of Literary and Artistic Works, Patent Cooperation Treaty (PCT) which facilitates obtaining of patents in several countries by filing a single application, World Trade Organization (WTO), Trade Related Aspects of Intellectual Property (TRIPS), Madrid system for the international registration of marks, The Hague system for the international deposit of industrial designs, Budapest treaty on the international recognition of the deposit of microorganisms for the purpose of patent procedure, International convention for the protection of new varieties of plants.

IPR - 03: Patent Search

What is a patent search. Who needs a patent search. Patent Search Types and Methodologies, Novelty Searches, Validity Searches, Infringement Searches, State-of-the-art searches.

Searching in Patent Databases:

Free search databases: USPTO, EPSPACE, WIPO, FreePatentsOnline, FreshPatents and JSPTO, Paid search databases: Micropat, Delphion, DialogPro, Patent Optimiser, Aureka and PatentCafe, Structure based search: STN search, SciFinder

IPR - 04: IP Reports Generation

Novelty search reports, Infringement search reports, Prior-art search reports, Patent invalidation reports, Competitive search reports, and Business analysis reports, Patent Filing and Drafting, Patent filing procedures, Indian patent act, patent drafting, PCT applications, provisional and complete specifications

References

1. Fundamentals of Jurisprudence by Dhyani, Allahabad Publication, Central Law.
2. Jurisprudence of Legal Theory by Dwivedi S.P. Allahabad Central Law Agency.
3. Text Book on Jurisprudence by Hilari WC Cobrey, Oxford Publications.
4. Treaties on Intellectual Property Rights by Blackstone
5. W.T.O. by Myneni, Asia Law House.
6. W.T.O. by Vasudeva, Minerva Publications, Delhi.
7. Law of Practice of Intellectual Property in India by Vikas Vashistha, Bharat Law Publications, Delhi.
8. Intellectual property rights by B L Wadhera, Universal Law Publications.
9. Trade Marks Act by Mittal, Eastern Book Company.
10. Patent Law by Narayana P, Eastern Book Company.
11. Intellectual Property Rights by Cornish, Universal Publications.

Paper II
Elective II: 1002
1002(E1): Green Chemistry
1002(E2): Pharmaceutical Analysis
1002(E3): Pharmaceutical design, development and computer application

E1: Green Chemistry

GC- 01: Introduction to Green Chemistry
GC-02: Approaches to green synthesis
GC-03: Microwave Induced and ultrasound assisted green synthesis
GC-04: Organic synthesis in aqueous phase and in solid state

GC-01: Introduction to Green Chemistry. 15 Hrs

Introduction. Principles, atom economy and scope. Inception to green chemistry. Introduction to alternative approaches. Solvent free reactions-principle, scope, utility of solvent free conditions, controlling solvent free reactions. Phase changes. optimum reaction temperatures, miscibility of reactants and catalysts. Solvent free microwave assisted organic synthesis: Introduction, solvent free techniques- Reactions on solid mineral supports, solid-liquid phase- transfer catalysts- Reactions without solvent support or catalyst. Microwave activation-benefits, limitations, equipment, microwave effects- according to reaction medium and according to reaction mechanism. Examples of reactions on solid supports, PTC, reactions without:support or catalyst.

GC-02: Approaches to green synthesis 15 Hrs

Basic principles of green synthesis. Different approaches to green synthesis a)Use of green reagents in green synthesis — Dimethyl carbonate, polymer supported reagents — peracids, chromic acid, PNBS, polymer supported peptide coupling reagents. b)Green catalysts-Acid catalysts- oxidation catalysts, basic catalysts, polymer supported catalysts. c)Phase-transfer catalysts in green synthesis-Aliquat 336, Benzyl trimethyl ammonium chloride or bromide (TMBA), TEBA, Tetra-n-butyl ammonium chloride, bromide, chlorate or hydroxide, benzyl triphenyl phosphonium iodide. Advantages of PTC reactions to green synthesis Application of PTCs in C-alkylation, N-alkylalion, S-alkylation, Darzens reaction, Williamsons synthesis, Wittig reaction. Heterocyclic compounds:3-alkyl coumarins, flavones, benzoxazines; Oxidation using H2O2 under PTC conditions. Use of Crown ethers in esterification, saponification , anhydride formation, aromatic substitution and elimination reactions.d)Ionic liquids as green solvents:-green solvents, reactions in acidic ionic liquids and in neutral ionic liquids (Hydrogenation, Diels-Alder reaction, o-alkylation and Nalkylation, methylene insertion reactions.) Synthesis of pravadoline

GC-03: Microwave induced and ultrasound assisted green synthesis 15 Hrs

a)Introduction to synthetic organic transformation under microwave i) Microwave assisted reactions in water — Hoffmann elimination, hydrolysis, oxidation, saponification reactions. ii) Microwave assisted reactions in organic solvents — Esterification reactions, Fries rearrangement Orthoester Claisen rearrangement, Diels- Alder reaction, decarboxylation. iii) Microwave solvent free reactions (solid state reactions) — deacetylation, deprotection saponification of esters, alkylation of reactive methylene compounds, synthesis of nitriles from aldehydes, reductions. Ultrasound assisted reactions: introduction, substitution reactions, addition, oxidation, reduction reactions. (b) Biocatalysts in organic synthesis — introduction i) Biochemical oxidations and reductions (microbial)-production of fine chemicals, vitamins and arninoacids. ii) Recombinant DNA technology-restriction enzymes, use of plasmids and cosmids. Application to insulin, human growth hormone. iii) By micro organisms-production of pencillins, streptomycin and chloramphenicol.

GC-04: Organic synthesis in aqueous phase and in solid state 15 Hrs

a)Aqueous reactions — Introduction, Diels-Alder reaction, Claisen rearrangement, Wittig-Homer reaction, Aldol condensation, Benzoin condensation. Oxidations — Epoxidation, dihydroxylation, oxidation of aldehydes and ketones, oxidation of arnines to nitro compounds. Reductions — Reduction of C-C double and triple bonds, reduction of carbonyl compounds and reduction of aromatic rings.b)Solid state reactions — Introduction, 1) Solid phase synthesis without using any solvent — halogenation, addition of HBr, Michael addition, dehydration of alcohols, aromatic substitution, reactions (bromination, nitration) ii) Solid supported synthesis — introduction, synthesis of (β-lactams, synthesis of pyrrole, furan, pyridines, imidazoles, coumarins and pyrimidines.

Recommended Books:

1. Organic synthesis in water. By Paul A. Grieco Blackie.
2. Green chemistry, Theory and Practical, Paul T.Anastas and John C.Warner.
3. New trends in green chemistry By V.K.Ahulwalia and M.Kidwai.
4. Organic Synthesis: Special techniques. V.K.Ahulwalia and Renu Aggarwal.

E2: Pharmaceutical Analysis

PA 01: Spectral Methods in Pharmaceutical Analysis
PA 02: Chromatography in Pharmaceutical Analysis-I
PA 03: Chromatography in Pharmaceutical Analysis-II
PA 04: Titrimetry, Chemical and Extraction methods in Pharmaceutical Analysis

PA 01: Spectral Methods in Pharmaceutical Analysis

(A) Ultraviolet and Visible Spectroscopy - Introduction. UV spectra of some representative drug molecules – Steroid enones, Ephedrine: the benzoid chromophore, ketoprofen: extended benzenechromophore, Procaine: amino group auxochrome, Phenyleprine: hydroxyl group auxochrome. Application of UV-Vis Spectrophotometry to Pharmaceutical quantitative Analysis – Assay of Frusemide in tablet, Assay of Penicillin by derivatization. Assay of 3 Drugs by i) Direct UV method ii) Suitable Chromogens and iii) Charge transfer Complexes. Difference spectrophotometry, Derivative Spectra, Applications of UV-Vis Spectrophotmetry in Pre - formulation and formulation.

(B) Infrared Spectroscopy - Introduction, Sample preparation, Application of IR Spectrophotomety in Structure Elucidation – interpretation of IR spectra of Paracetamol, aspirin, dexamethasone and phenoxymethyl pencillin potassium. Examples of IR Spectra of Drug molecules, IR Spectrophotometry as a fingerprint technique. Near IR analysis (NIRA) - Introduction, Examples of NIRA application – determination of particle size in United states Pharmacopia grade Aspirin, determination of blend uniformity, determination of active ingredients in multi-component dosage forms, moisture determination.

(C) Nuclear Magnetic Resonance Spectroscopy - Introduction, ^{1}H NMR – Application of NMR to Structure Confirmation in some drug molecules, ^{1}H NMR spectral analysis of Benzocaine, Phenacetin, Clofibrate and phenylephrine. ^{13}C NMR - ^{13}C NMR spectrum of Salbutamol sulphate, Two Dimensional NMR Spectra – Proton-proton correlation spectrum of Tranexamic acid. Application of NMR to Quantitative analysis.

PA 02: Chromatography in Pharmaceutica l Analysis-I

(A) Chromatography Theory, Classification of Chromatographic Methods, **Thin Layer Chromatography** – Introduction, Instrumentation, TLC Chromatogram, Stationary Phases, Eluotropic series and Mobile phases, Modification of TLC, Adsorbents, detection of compounds on TLC plate following development, Applications of TLC analysis – qualitative identity tests, limit tests. High performance TLC (HPTLC) – Applications of HPTLC – Assay for rifampicin (R) , isoniazid (I) and pyrazinamide(P).

(B) **High performance Capillary Electrophoresis** – Introduction, Instrumentation, control of separation. Application of capillary electrophoresis in pharmaceutical analysis – Separation of Atenolol and related impurities. Analysis of Non-steroidal anti-inflammatory drugs. Micellar Electrokinetic Chromatography – Analysis of flavonoids by MECC.

PA 03:Chromatography in Pharmaceutical Analysis-II

(A) **Gas Chromatography** –Summary of parameters governing capillary GC performance, Application of GC in quantitative analysis – Analysis of Methyl testosterone by internal standard method. Determination of manufacturing and degradation residues by GC – determination of pivolic acid in dipivefrin eye drops.. Determination of residual solvents. Application of GC in Bioanalysis. Gas Chromatography – Mass Spectrometry – Application of GC-MS to impurity profiling.

(B) **High Performance Liquid Chromatography** –
Applications of HPLC to the quantitative analysis of drugs in formulations –Assay of paracetamol and aspirin in tablets using a narrow range calibration curve, Assay of hydrocortisone cream with one point calibration against an internal standard. Assays involved in more specialized HPLC techniques – Assay of adrenaline injection by chromatography with an anionic ion-pairing agent. Liquid Chromatography – Mass Spectrometry – Application of LC-MS in pharmaceutical analysis.

PA 04: Titrimetry, Chemical and Extraction methods in Pharmaceutical Analysis

(A) Titrimetry and Chemical Methods - Introduction, Direct Acid/Base titrations in the aqueous phase, Indirect Titrations in aqueous phase – estimation of alcohols and hydroxyl values by reaction with acetic anhydride. Non-aqueous titrations – analysis of phenylephrine, Argentimetric Titrations – assays of Sodium chloride, potassium chloride, thiamine hydrochloride, mustin chloride and carbromal, Complexometric Titrations – metal salts estimations, Redox Titrations - assays of ferrous salts, hydrogen peroxide, sodium perborate and benzoyl peroxide by titration with $KMnO_4$, Iodometric Titrations – Asasy of phenolglycerol injection , Ion-pair Titrations, Diazotization Titrations – assay of sulphanilamide, Potentiometric Titrations – assay of Aspirin, Karl-Fischer Titrations, Automation of wet chemical methods, Application of FIA in Pharmaceutical analysis.

(B) Extraction Methods - Introduction, Commonly used excipients in formulations – (i)tablets and capsules (ii) suspensions and solutions (iii) creams and ointments. Solvent Extraction methods, (i) extraction of organic bases and acids utilizing their ionized and un-ionized forms. Partition between organic solvents, ion-pair extraction. Solid phase Extraction – Introduction, Methodology, types of adsorbents used in Solid phase Extraction – (i) Lipohilic silica gels. (ii) polar surfaced modified silica gels

Recommended Text Books:

1. Pharmaceutical Analysis by David G. Watson
2. Practical pharmaceutical chemistry Part I by Beckett & Stenlake
3. Pharmaceutical analysis by Ashtoshkar
4. Physical pharmacy by AN.Martin,J, Swarlbick etal
5. Biopharmaceutics and pharmacokinetics by Brahmanikar
6. Text book of physical pharmaceuticals by Subramaniyan
7. Inorganic pharmaceutical chemistry By Black
8. British Pharmacopoeia Vol I,II
9. Indian Pharmacopoeia Vol I,II
10. Bently's Text book of pharmaceutics by Rowlins
11. The science and practice of pharmacy by Remington

E3: Pharmaceutical design, development and computer application

PD - 01 : Principles of Drug Discovery
PD - 02 : SAR Studies
PD - 03 : QSAR Studies and Structure Based Drug Design
PD - 04 : Computational Chemistry and Molecular Modelling

PD - 01 : Principles of Drug Discovery

Drug discovery without lead – Pencillins and Librium. Lead discovery- random screening non-random screening.(screening of natural products, medical folklore, screening synthetic banks, existing drugs from natural ligand or modulator, combinatorial synthesis, computer aided designing & serendipity – in brief). Drug metabolism studies – phase I, Phase II metabolism. Clinical observations: phase I, phase-II, phase-III, phase -IV trials.(introductory treatment).Principles of drug design; agonist , antagonist drugs, structure pruning technique in drug design(eg. morphine pharmacophore). Development of cimetidine , captopril from lead molecules.

PD - 02: SAR Studies

1. Binding role of hydroxy group, Amino group, aromatic ring, double bond, ketones and amides. 2. Variation of substituents- alkyl substituents, aromatic substituents, extension of structure, chain extension/contraction, ring expansion/contraction, ring variation, ring fusion.Isosteres.iii. Simplification of the structure, rigidification, conformational blockers, X-ray crystallographic studies. Ex: A case study of Oxaminquine (schistosomiasis), Sulpha drugs(antibacterial),Benzodiazepines(Hypnotics) and Taxol analogues (anticancer drugs).

PD - 03: QSAR Studies and Structure Based Drug Design

QSAR parameters – Physiochemical parameters- Lipophilicity - Electronic parameters, Steric parameters, effect of electronic and steric parameters on lipophilicity. Methods used in QSAR studies- Linear free energy relationship (LFER) – Partial Least Squares Method - Multivariate Statistics – Correlation – Regression – Principal Component Analysis - Cluster significant analysis - Application of Hammet equation, Hansch analysis, significance of slopes and intercepts in Hansch analysis. QSAR- 2D, 3D**:** CoMFA, CoMSIA
Case study – on Pyranenamine. Achievements of QSAR – Forecasting biological activity, selection of proper substituents, bioisosterism, drug receptor interactions and pharmacokinetic information - Database similarity searches – Pair-wise alignment – Dot matrix comparison – Needleman -Wunsch Global sequence analysis – Smith waterman Local Sequence Alignment – Multiple Sequence Alignment – Homology Modeling – Energy minimization methods – Active site Identification – Virtual Screening – Small molecule Building – Docking Algorithms – Docking Analysis

PD - 04: Computational Chemistry and Molecular Modelling

Quantum mechanical and classical mechanical approaches - Empirical force field (Molecular mechanics)methods. Potential for bond stretching, bending, torsional, columbic and non bonded interactions. Coordinate systems – Z- matrix- Potential Energy Surface Contour Diagram- Minima, Maxima and Global Minimum, Local Minimum – Introduction to Molecular Mechanics - Features of Molecular Mechanics – Bond energy, bond angle energy, torsion angle energy, Charge-charge interaction-Bond Stretching – Angle Bending Torsional Terms – Improper Torsions and out of Plane Bending Motions – Cross Terms and Non Bonded Interactions – Electrostatic Interactions - Van-der Waals interactions - Hydrogen Bonding in Molecular Mechanics-

Force Field Equation in Energy minimization (Energy as function of r, θ, ω) and variation w.r.t ω only - Introduction to Derivative Minimization Methods – First Order Minimization – The steepest Descent Method – Conjugate Gradients Minimization – Conformation Search - Conformational Analysis of Ethane - Geometry optimization procedures - Introduction to molecular dynamics–description of molecular dynamics- basic elements of monte carlo method-differences between molecular dynamics and monte carlo method. Qualitative (brief) exposure to molecular dynamics simulations, conformational analysis.

Recommended books

1. Burger's medicinal chemistry and drug discovery. By Manfred E. Wolf.
2. Introduction to Medicinal chemistry. By Patrick.
3. Introduction to drug design. By Silverman
4. Comprehensive medicinal chemistry. Vol 1-5 By Hanzsch.
5. Principles of medicinal chemistry. By William Foye
6. Biochemical approach to medicinal chemistry. By Thomas Nogrady.
7. Pharmaceutical Chemistry and Drug synthesis By Roth and Kleeman

References

1. Drug design By E.J. Arienes
2. Jenkin's quantitative pharmaceutical chemistry By Knevel and Dryden
3. Recent advances in Bioinformatics By I. A. Khan and A Khanum
4. Computational chemistry By GH. Grant and WG. Richards
5. Molecular modelling By Hans Dieter Holtje and Gerd Folkers
6. Molecular modelling By Leach
7. Computational Chemistry by Jenson
8. Bio Informatics by Rastogi
9. The Science and practice of Pharmacy – Vol I and Vol II by Remington

Laboratory course
Project II