Parvatibai Chowgule College of Arts and Science

AUTONOMOUS

MARGAO - GOA

POST GRADUATE DEPARTMENT OF CHEMISTRY
M. Sc. ANALYTICAL CHEMISTRY

REVISED SYLLABUS

SEMESTER I

SEMESTER II

SEMESTER III

SEMESTER IV

EFFECTIVE FROM

ACADEMIC YEAR

2022 - 2023

M. Sc. ANALYTICAL CHEMISTRY COURSE STRUCTURE

SEMESTER	COURSES	CREDITS	HOURS
I AND II	**CORE COURSES**		
	PGM-CHE-AC-C401: Spectroscopy in Chemistry	3	36
	PGM-CHE-AC-C402: Laboratory Course in Analytical Chemistry	2	48
	PGM-CHE-IC-C401: General Inorganic Chemistry	3	36
	PGM-CHE-IC-C402: Laboratory Course in Inorganic Chemistry	2	48
	PGM-CHE-OC-C401: General Organic Chemistry	3	36
	PGM-CHE-OC-C402: Laboratory Course in Organic Chemistry	2	48
	PGM-CHE-PC-C401: General Physical Chemistry	3	36
	PGM-CHE-PC-C402: Laboratory Course in Physical Chemistry	2	48
	ELECTIVE COURSES		
	PGM-CHE-AO-E401: Analytical Techniques	2	24
	PGM-CHE-AO-E402: Electro analytical Techniques - I	2	24
	PGM-CHE-AO-E403: Electro analytical Techniques - II	2	24
	PGM-CHE-IO-E401: Topics in Inorganic Chemistry	2	24
	PGM-CHE-IO-E402: Environmental Control and Chemical Analysis	2	24
	PGM-CHE-OO-E401: Reaction Mechanisms in Organic Chemistry	2	24
	PGM-CHE-OO-E402: Reagents in Organic Synthesis	2	24
	PGM-CHE-OO-E403: Physical Organic Chemistry, Pericyclic and Photochemical Reactions	2	24
	PGM-CHE-PO-E401: Topics in Physical Chemistry	2	24
	PGM-CHE-PO-E402: Diffraction Methods	2	24
III AND IV	**CORE COURSES**		
	PGM-CHE-AC-C501: Fundamentals of Titrimetric Analysis	3	36
	PGM-CHE-AC-C502: Separation Techniques	3	36
	PGM-CHE-AC-C503: Spectral Methods of Analysis	3	36
	PGM-CHE-AC-C504: Experiments in Analytical Chemistry	3	72
	ELECTIVE COURSES		
	PGM-CHE-AO-E501: Advanced Mass Spectrometry	2	24
	PGM-CHE-AO-E502: Advanced NMR Spectroscopy	2	24
	PGM-CHE-AO-E503: Applied Analytical Chemistry	2	24
	PGM-CHE-AO-E504: Bio analytical Chemistry	2	24
	PGM-CHE-AO-E505: Calibrations and Validation	2	24
	PGM-CHE-AO-E506: Chemometrics	2	24
	PGM-CHE-AO-E507: Techniques in Chemical Analysis	2	24
	PGM-CHE-AO-E508: Thermal Methods of Analysis	2	24
	PGM-CHE-AO-E509: Quality Assurance and Quality Control in Analytical Chemistry	2	24
	PGM-CHE-AO-D510: Dissertation	8	192
	PGM-CHE-AO-M511: Modules in Experimental Chemistry	4	96
	PGM-CHE-AO-I512: Internship Module	4	96

M. Sc. PART I
CHEMISTRY
SEMESTER I AND II

CORE COURSES

Course Code: PGM-CHE-AC-C401
Course Title: Spectroscopy in Chemistry
Credits: 3
Duration: 36 Hours
Maximum Marks: 75

Course Objectives:
1. To enable students to identify and characterize the samples
2. To enable students to identify the organic compounds using spectroscopic methods

Course outcomes:
On successful completion of the course, the student will be able to:
CO1: Have an understanding on the different spectroscopic methods in chemistry
CO2: Identify and characterize organic compounds using spectroscopic methods

UNIT I: Introduction to Infrared Spectroscopy 12 Hours
Infrared spectroscopy- introduction, infrared absorption and molecular structure; near- Infrared spectrometry; molecular vibrations, factors influencing Vibrational frequencies; instrumentation of FTIR and sampling techniques; characteristic Vibrational frequencies of various functional groups and frequency shifts associated with structural changes.

UNIT II: NMR Spectroscopy 12 Hours
Introduction, theory, instrumentation; chemical shift, factors influencing chemical shift; solvents used in NMR; theory of spin-spin splitting and simple spin systems, AB, A_2B_2,A2B3; factors influencing coupling constant; introduction and principle to ^{13}C; off resonance decoupled spectra.

UNIT III: Mass Spectrometry, various techniques for structure determination 12 Hours
Basic principles; instrumentation; isotope abundances; molecular ion; Metastable ions; fragmentation processes; fragmentation associated with simple components like alcohols, amines, alkenes, simple aromatic and aliphatic hydrocarbons, Aldehyde, Ketones, halogen compounds; structure elucidation using UV-VIS, IR, NMR, mass spectra.
Note: Numerical are to be solved from above units

TEXT BOOK:

1. Spectroscopy of Organic Compounds, P. S. Kalsi; 2nd Edition, New Age International.

REFERENCE BOOKS:

1. Instrumental Methods of Chemical Analysis; G. W. Ewing, 5th Edition, McGraw-Hill
2. Instrumental Methods of Chemical Analysis, H. H. Willard, L. L. Merritt, J. A. Dean, F. A. Settle; 7th Edition CBS Publishing New Delhi
3. Analytical Chemistry: Principles, J. H. Kennedy, 2nd Edition, Saunders College Publishing
4. Organic Chemistry, R. T. Morrison, R. N. Boyd; 4th Edition, Prentice Hall India
5. Organic Spectroscopy, William Kemp, Palgrave; 3rd Edition
6. Spectrometric Identification of Organic Compounds, R. M. Silverstein, and F. X. Webster; 6th Edition, Wiley India.
7. Introduction to Spectroscopy, D. L. Pavia, G. M. Lampman; 4th Edition, Brooks/Cole

WEB REFERENCES:

1. http://www.chem.ucalgary.ca/courses/350/Carey5th/Ch13/ch13-ir-1.html
2. https://www.sciencedirect.com/topics/agricultural-and-biological-sciences/infrared-spectroscopy
3. https://www.sciencedirect.com/topics/materials-science/atomic-absorption-spectrometry
4. https://www.cis.rit.edu/htbooks/nmr/inside.htm

Course Code: PGM-CHE-AC-C402
Course Title: Laboratory Course in Analytical Chemistry
Credits: 2
Duration: 48 Hours
Maximum Marks: 50

Course Objectives:

1. To provide students with an overview of the different analytical techniques for analysis

Course Outcomes:

On successful completion of the course, the student will be able to:
CO1: Handle and use various analytical instruments
CO2: Understand the quantitative approach towards various instruments
CO3: Perform qualitative and quantitative analysis
CO4: Develop good laboratory practices, both conceptually and practically

I. UV-visible Spectrophotometer

1. To estimate the amount of D-glucose in given solution using Anthrone reagent
2. To determine the molar absorptivity of $KMnO_4$ and $K_2Cr_2O_7$ and simultaneously determine the amount of Manganese and Chromium in the solution
3. To estimate the amount of chloride by spectrophotometry using mercury (II) thiocyanate method

II. Flame Spectrophotometer

4. To estimate amount of Na/K from the given sample

III. Thermal Studies

5. TG-DTA studies on $CaC_2O_4.H_2O$
6. TG-DTA studies on $CuSO_4.5H_2O$
7. TG-DTA studies on Zn EDTA
8. DSC study on pharmaceutical product

IV. Volumetric Method

9.To estimate the amount of Aluminium, Calcium and Magnesium from pharmaceutical sample

V. Ion Exchange Chromatography

10. To separate and estimate the amount of Ni and Co from the given mixture
11. To separate and estimate the amount of chloride and bromide from the given mixture

VI. Solvent Extraction

12. To extract copper as copper dithiocarbamate (DTC) from $CuSO_4$ using solvent extraction and estimate the amount of copper by spectrophotometric method.
13. To extract copper from $CuSO_4$ as neocuproin complex by solvent extraction and estimation by spectrophotometric method.

VII. Conductometric Titration

14. To study all types of strong and weak acids and bases titrations by conductometric method using standard 0.1 N strong and weak acids and bases solution.

Note: Any Twelve experiment to be performed

REFERENCE BOOKS:

1. Analytical Chemistry, G. D. Christian; 5th Edition, John Willey and Sons
2. Vogel's Textbook of Quantitative Inorganic Analysis, 6th Edition, Pearson Education, Asia
3. Collection of Interesting Chemistry Experiments, A. J. Elias, University Press
5. Quantitative Analysis, Day and Underwood; 6th Edition, Prentice Hall
6. Analytical Chemistry for Technicians, John Kenkel; 3rd Edition, Lewis Publishers

VIDEO REFERENCES:

1. https://www.youtube.com/watch?v=wFpLgDceBhk
2. https://www.youtube.com/watch?v=idqG4G67Vv8
3. https://www.youtube.com/watch?v=w4WIKaMlLkE\

Course Code: PGM-CHE-IC-C401
Course Title: General Inorganic Chemistry
Credits: 3
Duration: 36 Hours
Maximum Marks: 75

Course Objectives:

1. To enable students to know about the atomic structure, different properties of atom and elemental chemistry
2. To enable students to study the fundamentals of Inorganic Chemistry

Course Outcomes:

On successful completion of the course, the student will be able to:
CO1: Identify different complexes and symmetry elements
CO2: Understand the importance of elements in biological systems
CO3: Understand molecular orbital theory for various molecules
CO4: Predict geometry of various molecules

UNIT I: Atomic and Molecular Structure, Bonding and Solid State Chemistry 12 Hours

Atomic Structure- Recapitulation; Atomic parameters: Atomic and ionic radii, ionisation energy, electron affinity, electro negativity; Molecular structure and bonding: Lewis structures and bond properties; the VSEPR theory; Valence bond theory- hydrogen molecule, homonuclear diatomic molecules, polyatomic molecules, hybridization; Molecular Orbital Theory: approximations of the theory (LCAO-MO), bonding and anti-bonding orbitals, homonuclear and heteronuclear diatomic molecules; Solid State Chemistry- packing of spheres: unit cell and description of crystal structure; close packing of spheres; holes in closed-packed structures; structures other than closed packed; ionic solids: characteristic structures of ionic solids, the rationalization of structures, defects in crystals.

UNIT II: Molecular Symmetry, Boron and Coordination Chemistry 12 Hours

Symmetry elements and symmetry operations; equivalent symmetry elements and equivalent atoms; point groups; symmetry point groups with examples; systematic procedure for symmetry classification of molecules with illustrative examples; dipole moment; Boron- introduction, borane, carboranes, Borazine; Coordination Chemistry- Recapitulation; shapes of coordination compounds; stereochemistry of coordination compounds. bonding in coordination compounds- valence bond theory and crystal field theory; stability constants of complexes and their determination; magnetism in coordination compounds; colour of coordination compounds; reaction mechanism of transition metal complexes.

UNIT III: Bioinorganic and Organometallic Chemistry **12 Hours**

Bioinorganic Chemistry- metal ions in biological systems; proteins and their functions- Heme proteins, synthetic oxygen carriers, electron transfer proteins-cytochromes, metalloproteins as enzymes-carboxypeptidase and Vitamin B12 coenzyme; chlorophyll and its use inphotosynthesis; Organometallic Chemistry- definition, classification of organo-transition metal complexes; synthesis, structure and bonding; the EAN, 18-electron and 16-electron rules; structure, bonding and important reactions of metal carbonyls; organometallic reagents in organic synthesis; application in homogeneous catalytic reactions (hydrogenation, hydroformylation, isomerisation and polymerisation), pi-metal complexes, activation of smallmolecules by coordination.

TEXT BOOK:

1. Inorganic Chemistry, D. F. Shriver and P. W. Atkins; 5th Edition, Oxford University Press
2. Principles of Bioinorganic Chemistry, Stephen J. Lippard and J. M. Berg; University Science Books

REFERENCE BOOKS:

1. Inorganic Chemistry: Principles of Structure and Reactivity, J. E. Huheey, E. A. Kiter; 4th Edition, Addison-Wesley Publishing House
2. Advanced Inorganic Chemistry, F. A. Cotton and G. Wilkinson; 6th Edition, Wiley Eastern, New Delhi
3. Theoretical Inorganic Chemistry, M. C. Day and J. Selbin; 2nd Edition, VanNostrand-Reinhold, New York
4. Nature of Chemical Bond, L. Pauling; 3rd Edition, Cornell University Press
5. Coordination Chemistry, D. Banerjea; Tata McGraw-Hill, New Delhi
6. Concise Inorganic Chemistry, J. D. Lee; 5th Edition, Chapman and Hall
7. Basic Inorganic Chemistry, F. A. Cotton and G. Wilkinson; 3rd Edition, John Wileyand Sons, Singapore
8. Principles of Solid State Chemistry, H. V. Keer; New Age International Ltd, New Delhi
9. Solid State Chemistry, D. K. Chakrabarty; 2nd Edition, New Age Publishers
10. Solid State Chemistry and Its Applications, A. R. West; John Wiley and Sons,Singapore

WEB REFERENCES:

1. https://en.wikiversity.org/wiki/Atomic_structure
2. https://www.britannica.com/science/atom/Atomic-mass-and-isotopes
3. https://chem.libretexts.org/Bookshelves/Inorganic_Chemistry/Supplemental_Modules_(Inorganic_Chemistry)/Coordination_Chemistry
4. http://www.chemistry.wustl.edu/~edudev/LabTutorials/naming_coord_comp.html
5. https://www.toppr.com/guides/chemistry/coordination-compounds/bonding-in-metal-carbonyls/

Course Code: PGM-CHE-IC-C402
Course Title: Laboratory Course in Inorganic Chemistry
Credits: 2
Maximum Marks: 50
Duration: 48 Hours

Course Objectives:

1. To enable students for preparing various coordination compounds and determine its purity.
2. To enable students for analyzing various inorganic analytes through various methods.

Course Outcomes:

On successful completion of the course, the student will be able to:

CO1: Understand the chemistry of coordination compounds
CO2: Perform quantitative analysis for various coordination compounds
CO3: Quantitatively detect various metal ions from coordination compound
CO4: Quantitatively analyse metal ion by spectrophotometry

Preparation and Characterisation of following Complexes

1. $K_3[Cr(SCN)_6].4H_2O$
2. $K_3[Cr(C_2O_4)_3]$ and estimate volumetrically the oxalate in the complex
3. Solid phase synthesis of trans-bis glycinato copper (II)
4. Potash alum from scrap aluminium (at micro scale level); to calculate the yield andpercent purity
5. To prepare Mohr's salt and determine the number of water molecules of crystallizationby titrating against potassium permanganate solution.

Quantitative Estimations

6. To estimate the amount of Calcium from Calcite ore
7. To estimate the amount of Copper in Gun Metal alloy or Devarda's alloy by using Iodometric method
8. To titrate the Zn(II) ion by $K_4[Fe(CN_6)]$ and verify the composition of the complex $K_3Zn_3[Fe(CN)_6]_2$
9. To estimate the amount of Cu/Fe/ Zn from the soil sample by AAS method
10. To determine the amount of copper from copper ammonia complex by the spectrophotometric method
11. To determine the amount of phosphate from water sample by heteropoly blue method
12. To determine the amount of total chromium from water sample using 1, 5- diphenyl carbazide by spectrophotometry

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REFERENCE BOOKS

1. Vogel's Text Book of Quantitative Chemical Analysis; 3rd and 4th Edition
2. Handbook of preparative Inorganic Chemistry; G. Brauer, Volume: 1 and 2

Course Code: PGM-CHE-OC-C401
Course Title: General Organic Chemistry
Credits: 3
Duration: 36 Hours
Maximum Marks: 75

Course Objectives:

1. To develop the knowledge in students on the concepts of topicity, prostereoisomerism and chemo-, regio- and stereoselectivity in organic reactions
2. To develop the knowledge in students on reaction mechanisms of various organic synthesis

Course Outcomes:

On successful completion of the course, the student will be able to:
CO1: Identify the presence or absence of aromaticity in organic compounds
CO2: Understand and apply various concepts in stereochemistry
CO3: Propose plausible mechanism of organic reactions
CO4: State various addition and elimination reactions

UNIT I: Stereochemistry **12 Hours**

Configurational nomenclature: *R* and *S*; D- and L-; *E* and *Z*; *cis* and *trans*; *syn* and *anti*-nomenclature; chirality in molecules with two and more chiral centres; conformational analysis of open chain compounds; *erythro* and *threo* nomenclature; structure, conformation and stereochemistry of monocyclic cycloalkanes (cyclopropane, cyclobutane, cyclopentane,

cyclohexane, cycloheptane and cyclooctane) with simple substituents; topicity and pro stereoisomerism-topicity of ligands and faces; homotopic, enantiotopic and diastereotopic ligands and faces; chemoselective, regioselective and stereoselective reactions; stereochemistry of *cis*- and *trans*-decalins; conformation and reactivity of cyclohexane, substituted cyclohexanes 'stereochemistry of cyclohexene and cyclohexanone', 2-alkyl and 3- alkyl ketone effect; introduction to stereochemistry of compounds containing N, S and P.

UNIT II: Reaction Mechanism **12 Hours**

Generation, structure, stability and reactivity of carbocations, carbanions, free radicals, carbenes and nitrenes; types of- reactions, mechanisms; thermodynamic and kinetic- control and control; the Hammond postulate and principle of microscopic reversibility; methods for determining reaction mechanisms like identification of products; determination of the presence of intermediates (isolation, detection, trapping and addition of suspected intermediate); isotopic labeling; stereochemical evidence; kinetic evidence and isotope effect (sufficient reactions to exemplify each method to be studied).

UNIT III: Addition to carbon-carbon multiple bonds; elimination reactions **12 Hours**

Mechanism and stereochemistry of addition reactions involving electrophiles, nucleophiles and free radicals; addition of HCl, HBr, HI, HOH, R-OH, NH_3, H_2SO_4, and halogen Br_2 to carbon-carbon double and triple bonds in open chain and cyclic compounds; addition of H_2 to C-C multiple bonds; hydroboration-oxidation and oxymercuration/demercuration; elimination reaction-the E2, E1 and E1cb mechanisms; orientation of the double bond, Saytzeff and Hofmann rule; effects of changes in the substrate, base, leaving group and medium on overall reactivity; comparison between E1, E2 and E1cb;elimination verses substitution; mechanism and orientation in pyrolytic syn elimination; various examples involving cyclic and acyclic substrates.

TEXT BOOK:

1. Advanced Organic Chemistry Reaction, Mechanism and Structure, J. March; 4th Edition, John Wiley

REFERENCE BOOKS:

1. Stereochemistry and Chemistry of Natural Products, I. L. Finar; ELBS, Longmans
2. Stereochemistry, M. Potapov, MIR Publishers, Moscow
3. Organic Chemistry, F. A. Carey
4. Organic Chemistry, S. H. Pine; 5th Edition, McGraw-Hill International
5. Advanced Organic Chemistry, F. A. Carey, R. J. Sundberg; Vol I and II, Plenum Press
6. Fundamentals of Organic Reaction Mechanisms, M. Hamis, Carl C. Wamser; John Wileyand Sons
7. Organic Chemistry- A Concise Approach, F. M. Menger, D. J. Goldsmith and L. Mendell
8. Organic Laboratory Techniques, R. J. Fessenden, J. S. Fessenden; Brookes/Cole Publishing Company
9. Stereochemistry of Organic Compounds- Principles and Application, D. Nassipuri; 2nd Edition, Wiley Eastern Limited
10. Mechanism and Structure in Organic Chemistry, E. S. Gould et al.
11. Stereochemistry of Carbon Compounds, E. L. Eliel, Tata McGraw-Hill.
12. J. Clayden, N. Greeves, S. Warren, P. Wothers, Organic Chemistry, Oxford University Press.

WEB REFERENCES:

1. https://www.sciencedirect.com/topics/chemistry/stereochemistry
2. https://www.sciencedirect.com/topics/chemistry/detailed-reaction-mechanisms
3. http://web.chem.ucla.edu/~harding/notes/notes_14D_additionpibonds.pdf
4. http://www.chem.ucalgary.ca/courses/350/Carey5th/Ch05/ch5-4.html.

5. https://www.khanacademy.org/science/organic-chemistry/stereochemistry-topic
6. https://www.khanacademy.org/science/organic-chemistry/alkenes-alkynes/alkene-reactions/v/introduction-to-reaction-mechanisms
7. https://www.khanacademy.org/science/organic-chemistry/substitution-elimination-reactions/elimination-reactions-tutorial/v/e2-reactions

Course Code: PGM-CHE-IC-C402
Course Title: Laboratory Course in Organic Chemistry
Credits: 2
Duration: 48 Hours
Maximum Marks: 50

Course Objectives:
1. To enable the students to apply certain theoretical concepts experimentally
2. To provide students with hands on experience on the basic laboratory techniques required for organic syntheses.

Course Outcomes:
On successful completion of the course, the student will be able to:
CO1: Gain the understanding of stoichiometric requirements during organic syntheses
CO2: Understand safe and good laboratory practices, handling of equipment
CO3: Learn common laboratory techniques including aqueous extraction
CO4: Synthesise the studied organic compounds and purify them.

I. Organic Synthesis
1. Aliphatic electrophilic substitution: Preparation of iodoform from ethanol and acetone
2. Aromatic electrophilic substitution: Preparation of p-bromo acetanilide
3. Oxidation: i. Benzoic acid from toluene
   ii. Iso-borneol to camphor using Jones reagent
4. Preparation of Cyclohexanone from cyclohexanol
5. Reduction: p-nitrophenyl methyl carbinol from p-nitro acetophenone by $NaBH_4$ and purification of the product through distillation under reduced pressure
6. Bromination of an alcohol using KBr/ $KBrO_3$ (at micro scale level)
7. Aldol condensation: Di benzal acetone from Benzaldehyde
8. Cannizzaro reaction using 4-chlorobenzaldehyde as substrate
9. Catalytic reduction of 1,4-benzoquinone to hydroquinone using H_2 over Pd/C.
10. Benzhydrol from benzaldehyde (Grignard reaction)
11. Cis-trans isomerisation of Stilbene and separation on UV-TLC
12. Purification techniques:
    i) a) Recrystalisation
       b) Distillation
    ii) a) Sublimation
       b) Steam distillation
13. Reduction of benzophenone with sodium borohydride.
14. Seperation Technique: Thin layer chromatography (ortho para meta Nitrophenols)
15. i.Reaction rate of SN2 reactions as a function of substrate structure
    ii. Reaction rate of SN1 reactions as a function of substrate structure
    iii. Secondary steric effects on SN2 reactions
    iv. Effect of leaving group on an SN2 reaction
    v. Effect of leaving group on an SN1 reaction

II. Extractions of:
13.i. Cinnamaldehyde from cinnamon sticks
   ii. Clove oil from Cloves

Note: Any twelve experiments to be performed

REFERENCE BOOKS:

1. Experiments and Techniques in Organic Chemistry, D. Pasto, C. Johnson and M. Miller; Prentice Hall
2. Organic Experiments, K. L. Williamson, D. C. Heath
3. Experimental Organic Chemistry, Vol I and II, P. R. Singh, D. S. Gupta, K. S. Bajpai; Tata McGraw-Hill
4. Laboratory Manual in Organic Chemistry, R. K. Bansal; Wiley Eastern.
5. Green Chemistry, Samuel Delvin; IVY Publishing House, Delhi
6. Organic Chemistry Laboratory, O. R. Rodig, C. E. Bell Jr. and A. K. Clark; Saunders College Publishing, New York
7. Organic Analytical Chemistry, Jag Mohan; Narosa Publishing House, New Delhi
8. Vogel's Textbook of Practical Organic Chemistry, 5th Edition; Brian S. Furniss, Antony J. Hannaford, Peter W. G. Smith, Austin R. Tatchell.
9. Elementary practical Organic Chemistry, Part 1: Small Scale Preparations Second Edition ; Arthur I. Vogel.
10. Experimental Organic Chemistry, Principles and Practice; Laurence M. Harwood & Christopher J. Moody, Blackwell Scientific Publications.

VIDEO REFERENCES:

1. https://www.youtube.com/watch?v=7g4e3dhtgjI
2. https://www.youtube.com/watch?v=Z6OyNB8V7Hc&t=383s

Course Code: PGM-CHE-PC-C401
Course Title: General Physical Chemistry
Credits: 3
Duration: 36 Hours
Maximum Marks: 75

Course Objectives:

1. To enable students to understand the mechanism of reactions
2. To enable students to understand the concept of micro-objects and its solutions throughquantum chemistry
3. To provide students with detail knowledge about thermodynamics and equilibrium systems

Course Outcomes:

On successful completion of the course, the student will be able to:
CO1: Apply the knowledge of thermodynamics
CO2: Propose the mechanism of different reactions taking place in the environment
CO3: Apply the knowledge of quantum chemistry to conjugated molecules
CO4: Apply the basic principle of miscibility of liquids

UNIT I: Quantum Chemistry **12 Hours**

Historical development of quantum theory, principle of quantum mechanics, wave particle duality, uncertainty principles, operators, functions, Eigen value equations, Schrodinger equation, application to simple system like free particle, particle in one dimensional, two dimensional and three dimensional box (quantization, separation of variables, degenerate wave functions); Hydrogen like atoms, Schrodinger equation and its solutions; atomic orbital wave function and interpretation; Hückel MO theory, secular equations, secular determinant, delocalization energy, charge density, pi-bond order, free valence, applications to C_2H_4, C_3H_5 (radical), C_4H_6, C_4H_4, C_6H_6, C_6H_8.

UNIT II: Thermodynamics and Phase Equilibria **12 Hours**

Thermodynamic properties- state and path properties; intrinsic and extrinsic properties, exact and

inexact differentials, internal energy, enthalpy, entropy, free energy and their relations and significances in predicting direction of chemical change; numerical on calculation of entropy; Gas laws, Real gases, Boyle temperature; partial molar quantities; Maxwell's relations; thermodynamic equations of state; third law of thermodynamics; need for third law; Nernst heat theorem, apparent exceptions to third law, application of third law.

Gibbs phase rule- Phase equilibria for two component systems forming solid solutions with and without maximum or minimum in freezing point curve, systems with partially miscible solid phases; phase equilibria for three component systems- graphical representation, three component liquid systems with one pair of partially miscible liquids; systems with two pairs and three pairs of partially miscible liquids, influence of temperature.

UNIT III: Chemical Kinetics and Polymers **12 Hours**

General introduction to various types of order of reaction including fractional order; comparative study of transition state and collision state theory (derivation not required); Eyring equation; free radical reactions, complex reactions like decomposition of acetaldehyde and ozone; reaction between H_2 and Br_2; homogeneous, heterogeneous and acid-base catalysis; autocatalysis and oscillatory reaction.

Polymers- introduction, types; molecular weight distributions; mechanism of free radical; determination of chain length; condensation polymerization; degree of polymerization from kinetic data (derivation not expected); polymers- conformers, thermodynamics; conducting polymers and applications.

NOTE: Numerical to be solved in possible units

TEXT BOOK:

1. Quantum Chemistry, Ira N. Levine

REFERENCE BOOKS:

1. Physical Chemistry, J. M. Castellan.
2. Chemical Kinetics, K. J. Laidler, Tata McGraw-Hill
3. Quantum Chemistry, R. K. Prasad, 3rd Edition, New Age International
4. Text Book of Physical Chemistry, K. L. Kapoor; Volume 1- 4; Macmillan India Limited
5. Physical Chemistry, P. W. Atkins and Julio De Paula, 8th Edition, Oxford University Press

WEB REFERENCES:

1. https://chem.libretexts.org/Bookshelves/Physical_and_Theoretical_Chemistry_Textbook_Maps/Supplemental_Modules_(Physical_and_Theoretical_Chemistry)/Kinetics/Modeling_Reaction_Kinetics/Transition_State_Theory/Eyring_equation
2. https://www.lenntech.com/library/ozone/decomposition/ozone-decomposition.htm
3. https://www.britannica.com/science/phase-rule

Course Code: PGM-CHE-PC-C402
Course Title: Laboratory Course in Physical Chemistry
Credits: 2
Duration: 48 Hours
Maximum Marks: 50

Course Objectives:

1. To give students an overview of different instruments and techniques used in Physical Chemistry laboratory

Course Outcomes:

On successful completion of the course, the student will be able to:

CO1: Handle instruments like conductometer, potentiometer and pH meter

CO2: Perform calculations through stoichiometry

Experiments:

1. To study the kinetics of hydrolysis of ethyl acetate and to determine: Energy of activation; Entropy of activation and Free energy change
2. To study the kinetics of the reaction between $K_2S_2O_8$ and KI and to determine: Energy of activation; Entropy of activation and Free energy change
3. To determine the order of reaction for the reaction between $K_2S_2O_8$ and KI by graphical, fractional change and differential methods
4. To determine the degree of hydrolysis and hydrolysis constant of a salt obtained from weak base and strong acid using conductometer
5. To determine the composition of a mixture containing acetic acid, monochloroaceticacid and hydrochloric acid by conductometric titration
6. To determine the equivalence point from derivative plot and determine the dissociation constants of a dibasic, malonic acid
7. To determine the equivalence point from the derivative plot and determine the dissociation constants the of a tribasic, phosphoric acid
8. To determine the formal redox potential from the derivative plot of Fe^{2+}/Fe^{3+} and Ce^{3+} $/Ce^{4+}$ system by potentiometric method
9. To study three component system of $C_6H_5CH_3$; C_2H_5OH and H_2O and obtain tie line
10. To study three component system of CH_3COOH; $CHCl_3$ and H_2O and obtain tie line
11. To study the: i. Phase of naphthalene and diphenyl system
    ii. Freezing point diagram of *o*-nitro phenol and *p*-toluidine
12. To determine the composition of a binary mixture (ethanol-water) from the viscosity-composition curve at room temperature by using viscometer

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REFERENCE BOOKS:

1. Practical Physical Chemistry, A. Finlay and J. A. Kitchener; Longman
2. Experimental Physical Chemistry, F. Daniels, J. H. Mathews; Longman
3. Practical Physical Chemistry, A. M. James, J. A. Churchil
4. Experimental Physical Chemistry, D. P. Shoemaker, C. W. Garland; McGraw Hill
5. Advanced Physical Chemistry, J. B. Yadav; Goel Publishing House, Meerut
6. Systematic Experimental Physical Chemistry, S. W. Rajbhoj, T. K. Chondhekar; Anjali Publication, Aurangabad

ELECTIVE COURSES

Course Code: PGM-CHE-AO-E401
Course Title: Analytical Techniques
Credits: 2
Duration: 24 Hours
Maximum Marks: 50

Course Objectives:

1. To provide knowledge to students about fundamentals of chromatography and its techniques in understanding the principle of separation

Course Outcomes:

On successful completion of the course, the student will be able to:

CO1: Know the fundamentals of chromatographic separations

CO2: Address modern challenges across the physical, chemical, and biological sciences and to isolate; examine the chemical and biological species as pure substances

CO3: Apply theoretical knowledge to design the practical for separation and analysis

CO4: Identify suitable chromatographic technique for separation of various compounds

UNIT I: Basics of Chromatographic Techniques **12 Hours**

Introduction; theory and principle of chromatographic technique, terms and parameters used in chromatography, plate and rate theory, classification of chromatographic methods, development of chromatogram, qualitative and quantitative analysis by chromatography; Paper Chromatography- introduction, principle, theory; types of paper chromatography; choice of solvent; applications; Thin Layer Chromatography- introduction; theory, principle; methodology, criteria for selection of stationary and mobile phases, choice of adsorbents, preparation and development of plates, identification and detection, reproducibility of Rf values, two-dimensional TLC, comparison of TLC with paper chromatography and column chromatography, applications; High Performance Thin Layer Chromatography- introduction, instrumentation, methodology, qualitative and quantitative analysis, applications.

UNIT II: Column, Partition, Adsorption and Ion Exchange Chromatography 12 Hours

Column Chromatography- definition, principle, types, column packing and sample loading, elution in column chromatography, experimental requirements, theory of development; migration rates of solutes; Partition Chromatography- introduction, theory, principle, movement of solute in chromatographic column, applications; Adsorption Chromatography- introduction, theory, principle, applications; Ion exchange chromatography- introduction, definition, principle, requirements for ion exchange resin, types of ion exchange resins,synthesis, basic features of ion exchange resins, factors affecting ion exchange equilibrium, packing of column, analysis of elute, resin properties- ion exchange capacity, resin selectivity, factors affecting the selectivity, applications.

TEXT BOOK:

Fundamentals of Analytical Chemistry, D. A. Skoog, D. M. West and F. J. Holler; 7th Edition, Sounders College Publishing.

REFERENCE BOOKS:

1. Analytical Chemistry, G. D. Christian; 5th Edition, John Wiley, New York
2. Principles of Instrumental Analysis, F. J. Holler, D. A. Skoog, S. R. Crouch; 6th Edition, Thomson Books/Cole
3. Analytical Chemistry: Principles, J. H. Kennedy; 2nd Edition, Saunders College Publishing
4. Vogel's Textbook of Quantitative Inorganic Analysis, J. Mendham, R. C. Denney, J. D. Barnes and M. Thomas; 6th Edition, Pearson Education Asia
5. Instrumental Methods of Analysis, H. H. Willard, L. L. Merritt, J. A. Dean, F. A. Settle; 7th Edition; CBS Publishing New Delhi
6. Instrumental Methods of Chemical Analysis, G. W. Ewing; 5th Edition, McGraw-Hill
7. Analytical Chemistry: Principles and Techniques, L. G. Hargis; Prentice Hall, New Jersey
8. Basic Concepts of Analytical Chemistry, S. M. Khopkar; Wiley Eastern.

WEB REFERENCES:

1. https://bitesizebio.com/29947/basics-chromatography-column/
2. https://www.studyread.com/column-chromatography/
3. Acikara, O. B. (2019). Ion-Exchange Chromatography and Its Applications. doi:10.5772/55744
4. https://lab-training.com/2021/03/26/paper-chromatography/
5. https://www.news-medical.net/life-sciences/How-Does-Ion-Exchange-Chromatography-Work.aspx

Course Code: PGM-CHE-AO-E402
Course Title: Electro analytical Techniques - I
Credits: 2
Duration: 24 Hours
Maximum Marks: 50

Course Objectives:

1. To enable the students to understand the theory of electro analytical chemistry
2. To incorporate the electrochemical measurements using a combination of problem-based learning approach to develop critical thinking skills in students

Course Outcomes:

On successful completion of the course, the student will be able to:

CO1: Comprehend the factors that must be controlled to obtain reliable and reproducibledata from electro analytical experiments

CO2: Identify the most appropriate electro analytical technique for a specific analysis

CO3: Design simple electrodes and determine their redox potentials to characterize electrodes

CO4: Draw redox cell diagram, cell notation and determine the cell potential

UNIT I: Potentiometry and Ion-selective electrodes 12 Hours

Basic concepts of potentiometers- electrochemical cell, reversible and irreversible cells, EMF series, standard electrode potential, Nernst equation, calculation of cell potential; introduction to potentiometer; metallic electrodes- electrodes of first and second kind; reference electrodes- hydrogen gas electrode, calomel, silver/silver chloride; types of potentiometric titrations; derivation of expression to calculate pH of solution through different cell constructions; precipitation and redox titration through cell constructions to determine the concentration of species under study; different method for determination of equivalent point, applications; theory of ion selective electrodes; membrane electrodes- classifications, properties; principle, design; membrane potential; selectivity; crystalline liquid membrane and enzyme electrodes; glass membrane electrodes; solid-state sensors; membrane gas- sensor.

UNIT II: Polarography, Electro gravimetry and Chrono methods 12 Hours

Introduction; basic theory and principle; deposition, dissolution and over potential,polarization of electrode; instrumentation of polarography, electrodes in polarography; advantages and limitations of dropping mercury electrode; supporting electrolytes; interference of oxygen, polarographic wave, half wave equation (derivation expected), Ilkovic equation and terms involved in it; polarographic maxima, half wave maxima; applications of polarography; numericals; Electro gravimetry- basic principles, completeness in deposition, composition of electrolyte, separation with controlled potentials, constant current electrolysis; Chrono methods- introduction, principle, methodology; applications of- chrono potentiometry, chrono coulometry.

Note: Numerical to be solved from above units

TEXT BOOK:

Fundamentals of Analytical Chemistry, D. A. Skoog, D. M. West, F. J. Holler; 7th Edition, Sounders College Publishing

REFERENCES BOOKS:

1. Analytical Chemistry, G. D. Christian; 5th Edition, John Wiley, New York
2. Principles of Instrumental Analysis, F. J. Holler, D. A. Skoog, S. R. Crouch; 6th Edition, Thomson Books/Cole
3. Analytical Chemistry: Principles, J. H. Kennedy; 2nd Edition, Saunders College Publishing
4. Vogel's Textbook of Quantitative Inorganic Analysis, J. Mendham, R. C. Denney, J. D. Barnes and M. Thomas; 6th Edition, Pearson Education Asia
5. Instrumental Methods of Analysis, H. H. Willard, L. L. Merritt, J. A. Dean, F. A. Settle; 7th Edition, CBS Publishing New Delhi
6. Instrumental Methods of Chemical Analysis, G. W. Ewing; 5th Edition, McGraw-Hill
7. Polarographic Methods in Analytical Chemistry, A. M. Bond
8. Instrumental Methods of Chemical Analysis, B. K. Sharma; Goel Publishing House.

WEB REFERENCES:

1. https://derangedphysiology.com/main/core-topics-intensive-care/arterial-blood-gas-interpretation/Chapter%205.0.2/ion-selective-electrode-membranes
2. http://www.federica.unina.it/agraria/analytical-chemistry/potentiometry/
3. https://chem.libretexts.org/Bookshelves/Analytical_Chemistry/Supplemental_Modules_(Analytical_Chemistry)/Analytical_Sciences_Digital_Library/JASDL/Courseware/Analytical_Electrochemistry%3A_Potentiometry
4. https://www.ias.ac.in/article/fulltext/reso/009/09/0051-0061
5. http://studymaterial.unipune.ac.in:8080/jspui/bitstream/123456789/8194/1/Introduiction%20to%20Electrogravimetry%20%281%29%20%281%29.pdf

Course Code: PGM-CHE-AO-E403
Course Title: Electro analytical Techniques - II
Credits: 2
Duration: 24 Hours
Maximum Marks: 50

Course Objectives:

1. To provide students with the basic understanding about the fundamental principles of voltammetry with rotating disk-ring electrodes, stripping voltammetry and amperometry
2. To demonstrate the experiments to students
3. To improve the basic understanding power of students for electro analytical techniques

Course Outcomes:

On successful completion of the course, the student will be able to:
CO1: Understand the basic concepts of electrodes
CO2: Understand physical and chemical properties of a material that can be studied by the commonly used electroanalytical techniques
CO3: Differentiate and compare different voltammograms
CO4: Apply theoretical concepts to analyse various metal ions quantitatively.

UNIT I: Amperometry and Voltammetry **12 Hours**

Amperometry- introduction to amperometric titrations, instrumentation, electric circuit, indicator electrodes, reference electrodes, types of amperometric titrations, advantages and disadvantages of amperometric titrations; applications; Voltammetry- introduction, theory, principle, excitation signals, instrumentation; working electrodes and modified electrodes; voltammogram; types of voltametric techniques, applications- oxygen sensor and enzyme- based sensor; cyclic voltammetry; applications of cyclic voltammetry, stripping voltammetry- anodic and cathodic stripping method, voltammetry with microelectrodes; applications of voltammetry-inorganic and organic analysis.

UNIT II: Coulometry and Karl Fischer Titration **12 Hours**

Coulometry- introduction, theory, determining electrical charge, current efficiency requirements, current measuring devices- hydrogen-oxygen coulometer, silver coulometer, iodine coulometer; coulometry at controlled potential; coulometry at constant current; variation in coulometric techniques; coulometric titrations- theory, instrumentation, comparison of coulometric titrations over conventional titrations, applications; Karl Fischer Titrations- introduction, theory, types; criterion in selection; methodology for determination of water content in samples and general sample requirement.

TEXT BOOK:

Fundamentals of Analytical Chemistry, D. A. Skoog, D. M. West and F. J. Holler; 7th Edition, Sounders College Publishing.

REFERENCES BOOKS:

1. Principles of Instrumental Analysis; F. J. Holler, D. A. Skoog, S. R. Crouch; 6th Edition, Thomson Books/Cole
2. Analytical Chemistry: Principles; J. H. Kennedy; 2nd Edition, Saunders College Publishing
3. Instrumental Methods of Chemical Analysis, B. K. Sharma; Goel Publishing House
4. Instrumental Methods of Chemical Analysis, H. H. Willard, L. L. Merritt, J. A. Dean, F. A. Settle; 7th Edition, CBS Publishing New Delhi
5. Instrumental Methods of Chemical Analysis, G. W. Ewing; 5th Edition, McGraw-Hill.
6. Analytical Chemistry, G. D. Christian; 5th Edition, John Wiley, New York.
7. Vogel's Textbook of Quantitative Inorganic Analysis, J. Mendham, R. C. Denney, J. D. Barnes and M. Thomas; 6th Edition, Pearson Education Asia.

WEB REFERENCES:

1. https://www.azom.com/article.aspx?ArticleID=16017
2. https://mcckf.com/english/kf-basic/what.html
3. https://chem.uiowa.edu/sites/chem.uiowa.edu/files/people/shaw/LUCIO%20GM%20KF-Titration%20March-2013.pdf
4. https://chem.libretexts.org/Bookshelves/Analytical_Chemistry/Book%3A_Analytical_Chemistry_2.1_(Harvey)/11%3A_Electrochemical_Methods/11.04%3A_Voltammetric_and_Amperometric_Methods
5. http://rxpharmaworld.blogspot.com/2016/12/coulometry.html

Course Code: PGM-CHE-IO-E401
Course Title: Topics in Inorganic Chemistry
Credits: 2
Duration: 24 Hours
Maximum Marks: 50

Course Objectives:

1. To provide students with an overview of important topics in Inorganic Chemistry
2. To provide students with in-depth knowledge of various inorganic elements

Course Outcomes:

On successful completion of the course, the student will be able to:
CO1: Understand the basics of acid and bases
CO2: Understand the chemistry of p-block elements, d-block elements, lanthanide andactinides
CO3: Understand the separation techniques related to inner transition elements
CO4: Understand the importance of f- block elements

UNIT I: Main group elements and their selected compound 12 Hours

A. Carbon group: allotropes of carbon, C60 and compounds (fullerenes), intercalation compounds of graphite, carbides, compounds of silicon- silanes, silicates and silicones, Zeolites; Nitrogen group: nitrogen activation, oxidation states of nitrogen and their inter conversion, PN and SN compounds; Oxygen group: oxy acids and oxo anions of S and N; halogen group: inter halogens, structures, properties and applications.
B. Oxy acids and oxo anions of halogens, compounds of noble gases.

UNIT II: Inner transition elements and Acid-Base Theory 12 Hours

A. Inner-transition elements: lanthanides and actinides- occurrence, properties, oxidation states, electronic structure, colour, spectra and magnetic properties; lanthanide contraction; compounds of lanthanides and actinides; separation techniques.
B. Arrhenius, Bronsted and Lewis Theory of acids and bases; Hard and soft acids and bases; HSAB principle and its applications.

TEXT BOOK:
Inorganic Chemistry, D. F. Shriver, P. W. Atkins; 5th Edition, Oxford University Press

REFERENCE BOOKS:
1. Inorganic Chemistry: Principles of Structure and Reactivity, J. E. Huheey, E. A. Kiter; 4th Edition, Addison-Wesley Publishing House
2. Chemistry of the Elements, N. N. Greenwood, A. Earn Shaw; Pergamon Press, Great Britain
3. Advanced Inorganic Chemistry, F. A. Cotton, G. Wilkinson, Hurillo, Bochmann; 6th Edition, Wiley Interscience
4. Concise Inorganic Chemistry, J. D. Lee; 5th Edition, Chapman and Hall
5. Basic Inorganic Chemistry, F. A. Cotton, G. Wilkinson, Paul L. Gaus; 3rd Edition, John Wiley and Sons

WEB REFERENCES:
1.https://www.britannica.com/science/carbon-chemical-element/Structure-of-carbon- allotropes
2. https://www.visionlearning.com/en/library/Chemistry/1/Acids-and-Bases/58
3.https://chem.libretexts.org/Bookshelves/Inorganic_Chemistry/Supplemental_Modules_and _Websites_(Inorganic_Chemistry)/Descriptive_Chemistry/Elements_Organized_by_Block/4 _f-Block_Elements/The_Lanthanides/aLanthanides%3A_Properties_and_Reactions
4.https://sciencenotes.org/main-group-elements-definition-and-importance/
5.https://www.britannica.com/science/zeolite

Course Code: PGM-CHE-IO-E402
Course Title: Environmental Control and Chemical Analysis
Credits: 2
Duration: 24 Hours
Maximum Marks: 50

Course Objectives:
1. To enable students to understand the sources, effects and mitigation of various types of pollution
2. To enable students for gaining knowledge on the procedure for analysis of greenhouse gases, pesticides, explosives, cosmetics and paints

Course Outcomes:
On successful completion of the course, the student will be able to:
CO1: Identify the sources and effects of various types of pollution
CO2: Describe the analysis of greenhouse gases
CO3: State the control measures of various pollutions
CO4: Describe the analysis of pesticides, explosives, cosmetics and paints

UNIT I: Air and Water Pollution **12 Hours**

A. Air Pollution- Introduction; sources of gaseous pollutants; classification; effects of air pollutants on living and non-living objects; sampling methods for gaseous, liquid and solid pollutants; greenhouse effect; acid rain; ozone depletion and their consequences on environment; major air pollution disasters; electrostatic precipitation; filters; problems in industrial area; method to control air pollution; air pollution problems in India.

B. Water Pollution- Introduction; types; sources and classification of water pollutants; toxic elements in water; mercury pollution; estimation of organo- mercurials; pesticides in water; potable and sanitary water; industrial water pollution; constituents of aquatic environment; oxygen content of water and aquatic life; effects of water pollutants on life and environment; method to control water pollution; analytical procedures for analyses of industrial waste water and treatment; aerobic and anaerobic aeration of water; principle of coagulation; flocculation;

softening; disinfection; demineralization; measurements of dissolved oxygen (DO), Chemical oxygen demand (COD), Biochemical oxygen demand (BOD), Total organic carbon (TOC).

UNIT II: Soil Pollution; paints and pigments; Analysis of insecticides, pesticides herbicides **12 Hours**

A. Soil Pollution- Introduction, classification of pollutants and their characteristics, sources, prevention and control; soil composition; organic and inorganic components in soil; degradation by natural sources; sources of pesticide residue in the soil, its effect on life; biochemical effect of pesticides; analytical techniques for pesticide residue analysis; Nitrogen and NPK in soil and water; instrumental techniques in environmental pollutant analysis.

B. Paints and Pigments- introduction to paints; pigment separation; identification of binder; identification and analysis of thinner, primers, pigments; binder and thinner of- latex paints, solvent type coatings; tests on total coating.

C. Analysis of insecticides and pesticides- Introduction; analysis of BHC, DDT, Malathion, Parathion, 2, 4-dichloro phenoxy acetic acid.

D. Analysis of herbicides- Introduction; dalapon, paraquat, Butacarb, Benomyl, Bordeaux mixture.

TEXT BOOKS:

Environmental Chemistry, A. K. De; New Age International Publishers

REFERENCE BOOKS:

1. Standard Methods of Waste and Wastewater Analysis, A. K. De
2. Environmental Chemistry, B. K. Sharma
3. Introduction to Air Pollution, P. K. Trivedi
4. Environmental Pollution Analysis, S. M. Khopkar
5. Standard Methods of Chemical Analysis, F. J. Welcher; Volume 3, Part-B
6. Environmental Chemistry, Garry. W. Vanloon; 3rd Edition, Oxford University Press

WEB REFERENCES:

1. https://www.sciencedirect.com/topics/chemistry/water-pollution
2. http://www.ncids.com/forensic/labs/Trace/Technical/3_PAINT.pdf
3. https://www.sepa.org.uk/media/120465/mtc_chem_of_air_pollution.pdf
4. https://www.sciencedirect.com/topics/engineering/soil-pollution
5. https://www.sciencedirect.com/book/9780080238463/the-analysis-of-explosives

Course Code: PGM-CHE-OO-E401
Course Title: Reaction Mechanisms in Organic Chemistry
Credits: 2
Duration: 24 Hours
Maximum Marks: 50

Course Objectives:

1. To enable students to understand electrophilic substitution reactions and mechanisms
2. To enable students to apply mechanistic concepts of nucleophilic addition to carbonyl group

Course Outcomes:

On successful completion of the course, the student will be able to:
CO1: Understand organic reactions and will be able to propose plausible mechanisms
CO2: Choose appropriate reagents to carry out substitution reactions
CO3: Understand the aromatic electrophilic and nucleophilic substitution reactions
CO4: Understand the aliphatic electrophilic and nucleophilic substitution reactions

UNIT I: Aliphatic Nucleophilic and Electrophilic Substitution Reactions **12 Hours**

The SN2, SN1, mixed SN1 and SN2 and SET mechanisms; neighbouring group mechanism,

neighbouring participation by π and σ bonds, anchimeric assistance; classical and non-classical carbocations, phenonium ions, norbornyl system, common carbocation rearrangements; the SNi mechanism; nucleophilic substitution at an allylic, aliphatic and vinylic carbon; reactivity effect of substrate structure, attacking nucleophiles, leaving group and reaction medium; bimolecular mechanisms- SE2 and SEi; SE1 mechanism; electrophilic substitution accompanied by double bond shifts; effects of substrates; leaving group and the solvent polarity on the reactivity.

UNIT II: Aromatic electrophilic and nucleophilic substitution reactions and addition to Carbon-Oxygen multiple bonds **12 Hours**

Introduction to general mechanisms involved, reactivity of arenes, product distribution; ipso attack and orientation in benzene with more than one substituent; Friedel-Crafts and related reactions- alkylation, acylation, formylation; Vilsmeier reaction, Gattermann-Koch reaction; Fries rearrangement and Prins reaction; diazotization, nitrosation, nitration, sulphonation, mercuration; introduction to addition-elimination mechanisms and elimination-addition mechanism in aromatic nucleophilic substitution; Ullmann reaction; Schiemann reaction; Von Richter reaction; Sommelet-Hauser rearrangement; Smiles rearrangement; Mechanism of condensation reactions involving enolates- Aldol, Knoevenegel, Claisen, Darzen, Stobbe, Perkin and Benzoin reactions; hydrolysis of esters and amides; aminolysis of esters.

TEXT BOOK:

Advanced Organic Chemistry Reaction, Mechanism and Structure, J. March; 4th Edition, John Willey

REFERENCE BOOKS:

1. Organic Chemistry, F. A. Carey
2. A Guidebook to Mechanisms in Organic Chemistry, P. Sykes; 6th Edition, PearsonEducation
3. Organic Chemistry, Clayden, Greeves and Warren; Oxford University Press
4. Mechanism and Structure in Organic Chemistry, E. S. Gould et al
5. Organic Chemistry, S. H. Pine; 5th Edition, McGraw-Hill International
6. Advanced Organic Chemistry, F. A. Carey and R. J. Sundberg; Vol. I and II

WEB REFERENCES:

1. https://www.organic-chemistry.org/namedreactions/nucleophilic-substitution-sn1-sn2.shtm
2. https://www.sciencedirect.com/topics/chemistry/nucleophilic-aliphatic-substitution
3. http://www.chem.ucla.edu/~harding/notes/notes_14D_EAS01.pdf
4. https://www.sciencedirect.com/topics/chemistry/electrophilic-aromatic-substitution
5. https://www.masterorganicchemistry.com/2018/08/20/nucleophilic-aromatic-substitution-nas/

Course Code: PGM-CHE-OO-E402
Course Title: Reagents in Organic Synthesis
Credits: 2
Duration: 24 Hours
Maximum Marks: 50

Course Objectives:

1. To provide students with knowledge of oxidation processes used in organic syntheses
2. To provide students with knowledge of reduction processes used in organic syntheses

Course Outcomes:

On successful completion of the course, the student will be able to:
CO1: Choose appropriate oxidizing agent for oxidation of a particular functional group
CO2: Choose appropriate reducing agent for reduction of a particular functional group
CO3: Propose the mechanism of reduction reactions
CO4: Propose the mechanism of oxidation reactions

UNIT I: Oxidation Reactions **12 Hours**

Oppenauer oxidation, aromatization and dehydrogenation, oxidation of hydroxyl group with Triphenyl bismuth carbonate, O_2/Pt catalyst, silver carbonate/celite, sodium bromate/CANand $NaOCl/CH_3COOH$; chromium and manganese compounds: oxidation of alcohols, aldehydes, C-C double bonds and C-H bonds in hydrocarbons; peracids and other peroxides; types of peracids and preparation; oxidation of C-C double bonds in acyclic and cyclic systems, carbonyl compounds, amines and sulphides, allylic C-H bonds and oxidation with molecular oxygen; other methods of oxidation involving periodic acid, Na/K metaperiodate, lead tetraacetate, mercuric acetate, selenium dioxide, osmium tetroxide, DMSO, thallium nitrate, DDQ, Prevost's reagent and Woodward conditions; ozonolysis, catalytic oxidation over Pt; photosensitised and palladium-catalysed oxidation of alkenes.

UNIT II: Reduction Reactions **12 Hours**

Catalytic hydrogenation- different catalysts, solvents and equipment; functional group reductions and homogeneous catalytic hydrogenation; reductions by hydride-transfer reagents and related reactions- MPV reduction, $NaBH_4$, $NaB(CN)H_3$, Trialkyl borohydrides, LAH and lithium hydrido alkoxy aluminates, mixed LAH-$AlCl_3$ reagents, DIBALH and Reductions with borane and dialkyl boranes; enzymatic reduction involving liver alcohol dehydrogenase/ NADH and Baker's yeast; other methods of reduction- Wolff-Kishner, Raney Ni desulphurisation, di-imide, low-valent titanium species, trialkyl tin hydrides and trialkylsilanes.

TEXT BOOK:

Some Modern Methods of Organic Synthesis, W. Carruthers; Cambridge University Press, Cambridge

REFERENCE BOOKS:

1. Modern Synthetic Reactions, Herbert O. House, W. A. Benjamin; 2nd Edition
2. Advanced Organic Chemistry Reaction, Mechanism and Structure, J. March; Mc GrawHill, International Books Company
3. Advanced Organic Chemistry, F. A. Carey, R. J. Sundberg; Vol I and II, Plenum Press

WEB REFERENCES:

1. https://www.organic-chemistry.org/namedreactions/meerwein-ponndorf-verley-reduction.shtm
2. https://www.organic-chemistry.org/namedreactions/wolff-kishner-reduction.shtm
3. https://www.organic-chemistry.org/namedreactions/prevost-reaction.shtm
4. https://chem.pg.edu.pl/documents/614792/2c6c0579-c52b-400e-a396-07a03363f4e0
5. https://www.organic-chemistry.org/namedreactions/oppenauer-oxidation.shtm

Course Code: PGM-CHE-OO-E403
Course Title: Physical Organic Chemistry, Pericyclic and Photochemical Reactions
Credits: 2
Duration: 24 Hours
Maximum Marks: 50

Course Objectives:

1. To enable students to understand the Physical Organic concepts in Organic Chemistry
2. To enable students to understand the Photochemical and Pericyclic chemistry

Course Outcomes:

On successful completion of the course, the student will be able to:

CO1: Understand what are molecular orbitals and how to use molecular orbital theory to understand reaction mechanisms

CO2: write mechanism for Photochemical and pericyclic reactions.

UNIT I: Molecular Orbitals, Delocalized Chemical Bonding, Structure and Reactivity

12 Hours

Molecular orbitals of simple acyclic and monocyclic systems, qualitative description; frontier orbitals; importance of FMOs in organic reactions; conjugation, cross conjugation, resonance, hyper conjugation and tautomerism; alternant and non-alternant hydrocarbons; aromaticity in benzenoid and non-benzenoid compounds; Huckel's rule; annulenes, aromatic, non-aromatic and antiaromatic compounds; Acidity and basicity- different concepts, HSAB concept and factors affecting it; effect of structure and medium on acid and base strength; concept of super acids and super bases; electrophilicity and nucleophilicity, ambident nucleophiles and electrophiles, concepts and examples; tautomerism- concept, tautomeric equilibrium, relation with isomerism; types of tautomerism including ring, chain tautomerism and valence tautomerism; proto tropic shift in different systems.

UNIT II: Pericyclic and Photochemical Reactions **12 Hours**

Pericyclic reactions- electrocyclization, cycloaddition, sigma tropic rearrangements and other related concerted reactions; Principles, applications of photochemical reactions in organic chemistry.

TEXT BOOKS:

1. Pericyclic Reactions, Ian Fleming, Oxford University Press
2. Molecular Orbitals and Organic Chemical Reactions, Ian Fleming, John Wiley and Sons

REFERENCE BOOKS:

1. Advanced Organic Chemistry Reaction, Mechanism and Structure, J. March; 4th Edition, John Willey
2. Fundamentals of Organic Reaction Mechanisms, M. Hamis, Carl C. Wamser, John Wiley and Sons
3. Organic Chemistry- A Concise Approach, F. M. Menger, D. J. Goldsmith and L. Mendell
4. Mechanism and Structure in Organic Chemistry, E. S. Gould et al

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1. https://www.sparknotes.com/chemistry/organic1/orbitals/section2/
2. https://chem.libretexts.org/Bookshelves/Organic_Chemistry/Supplemental_Modules_(Organic_Chemistry)/Reactions/Pericyclic_Reactions
3. https://www.chegg.com/learn/chemistry/organic-chemistry/pericyclic-reactions
4. https://www.khanacademy.org/science/organic-chemistry/conjugation-diels-alder-mo-theory

Course Code: PGM-CHE-PO-E401
Course Title: Topics in Physical Chemistry
Credits: 2
Duration: 24 Hours
Maximum Marks: 50

Course Objectives:

1. To enable students to study the physical behaviour and some chemical reactions under the influence of visible and ultraviolet light
2. To enable students to understand the concepts of magnetism
3. To enable students to understand the concept of electrode potential

Course Outcomes:

On successful completion of the course, the student will be able to:

CO1: Understand the magnetic behaviour of materials
CO2: Understand the difference between the over voltages
CO3: Use photochemistry principle in various areas like lasers, flash photolysis
CO4: Understand the various reaction like photo reduction and photo oxidation

UNIT I: Magnetochemistry **12 Hours**

Introduction to magnetism; types of magnetism- diamagnetism, paramagnetism, ferromagnetism, anti-ferromagnetism and ferrimagnetism; electron spin and magnetic moment; theory of diamagnetism; Langevins theory; magnetic susceptibility and its measurements- Guoy's and Quinke's method; Ranking's transition metal complexes; ferromagnetism- domain theory; hysteresis in magnetism; ferrimagnetism; magnetic anisotropy, magnetic exchange interactions; magnetic transition- Curie and Neel temperature; magnetic ceramic materials; applications of magnetic materials.

UNIT II: Electrochemistry and Photochemistry **12 Hours**

Electrochemistry- introduction; Polarization; method for elimination of polarization; decomposition potential; experimental determination of decomposition potential; overvoltage, hydrogen over voltage, oxygen over voltage, types of overvoltage, experimentaldetermination of over voltage, factors affecting the over voltage.

Photochemistry- absorption and emission radiation of photochemical interest (Einstein's derivation not expected); laws of photochemistry; Frank-Condon principle; Jablonski diagram illustrating fluorescence and phosphorescence; long range and short-range energy transfer process; photo oxidation; photo reduction; photosynthesis; photosensitised reactions; chemiluminescence, mechanism of chemiluminescence; flash photolysis and lasers.

Note: Numerical may be solved wherever possible for above units

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TEXT BOOKS:

1. Fundamentals of Photochemistry, K. K. Rohatgi-Mukherjee; Wiley Eastern, New Delhi
2. Magnetic susceptibility, L. N. Muley; Inter science Publishers, New York

REFERENCE BOOKS:

Instrumental Methods of Chemical Analysis, B. K. Sharma; Goel Publishing House

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1. http://www.irm.umn.edu/hg2m/hg2m_b/hg2m_b.html
2. https://www.google.com/url?sa=t&source=web&rct=j&url=https://www.britannica.com/science/polymer&ved=2ahUKEwitpqAx5HnAhVExTgGHQv8C24QFjAmegQIBxAB&usg=AOvVaw0-_N41elqjLur5vCql3p8z&cshid=1579501965101
3. http://www.ccl.net/cca/documents/dyoung/topics-orig/magnet.html
4. https://www2.chemistry.msu.edu/faculty/reusch/VirtTxtJml/photchem.htm

Course Code: PGM-CHE-PO-E402
Course Title: Diffraction Methods
Credits: 2
Duration: 24 Hours
Maximum Marks: 50

Course Objectives:

1. To give students an overview of diffraction methods in solid state chemistry for solving structural problem
2. To enable students to learn the use of excel in solving problems on X-ray diffraction

Course Outcomes:

On successful completion of the course, the student will be able to:
CO1: Understand the working of XRD

CO2: Interpret the XRD spectra
CO3: Handle the software like origin used in determination of crystal structure
CO4: Use Microsoft Excel to get X-ray analysis

UNIT I: X-ray diffraction analysis **12 Hours**

Introduction, packing of spheres - cubic and hexagonal close packing; radius ratio rule, unit cell, types of unit cells and their characteristics; description of crystal structure; Bravias lattice; Bragg's Law, powder method, single-crystal X-ray diffraction; principle, instrumentation, scope and limitations of the method; X-ray scattering factors; calculations of unit cell dimensions from powder diffraction patterns for cubic, tetragonal and orthorhombic systems; reciprocal lattice concept; X-ray intensity calculations to decide the ionic configurations.

UNIT II: Problem solving through diffraction methods **12 Hours**

Introduction to spreadsheet-based software; Microsoft Excel; development of spreadsheets for-some simple test cases like Gaussian curve (study the effect of standard deviation and centre of Gaussian), plotting of trigonometric functions like sin, cos and their linear combinations (Fourier synthesis for crystal structure determination); precise lattice parameter measurements; crystal structure determination- cubic; FCC, BCC, Hexagonal and other important crystal structure.

TEXT BOOK:

Solid State Chemistry and its Applications; A. R. West, John-Wiley and Sons,Chinchester

REFERENCE BOOKS:

1. X-ray diffraction: A practical Approach, C. Suryanarayana and M. Grant, Norton Plenum Press, New York
2. Elements of X- ray Diffraction, B. D. Cullity; Addison Wesley
3. Principles of Solid State Chemistry, H. V. Keer; New Age International Ltd, New Delhi

WEB REFERENCES:

1. https://www.originlab.com/Origin
2. https://books.google.co.in/books?id=vk9fnLH56DYC&printsec=frontcover&dq=powder+diffraction+theory+and+practice&hl=en&sa=X&ved=0ahUKEwisvu--mpHnAhXPyDgGHW3XDMoQ6AEIZzAJ#v=onepage&q&f=false
3. https://link.springer.com/chapter/10.1007/978-1-4614-3954-7_12
4. https://epdf.pub/queue/powder-diffraction-theory-and-practice.html

M. Sc. PART - II
ANALYTICAL CHEMISTRY
SEMESTER III AND IV

CORE COURSES

Course Code: PGM-CHE-AC-C501
Course Title: Fundamentals of Titrimetric Analysis
Credits: 3
Duration: 36 Hours
Maximum Marks: 75

Course Objectives:

1. To enable students to understand the concept of titrimetry
2. To enable students to understand fundamental concepts in acid-base, precipitation, complex formation, redox system

Course Outcomes:

On successful completion of the course, the student will be able to:
CO1: Determine equivalence point of various titrations theoretically
CO2: Make basic quantitative calculations regarding a number of chemical concepts
CO3: Write and understand chemical reactions and stoichiometry
CO4: Master the concepts like chemical equilibria, complexation, solubility, acidity andbasicity

UNIT I: Acid-Base Titrations **12 Hours**

Acid-Base titrations- introduction, theory of acid-base indicators; range of indicators; selection of proper indicator; indicator errors; colour change; neutralization curves for strong acid-strong base, weak acid-strong base and weak base-strong acid weak acid-weak base titrations; poly functional acids and bases; titration curves for mono and poly functional acids and bases; titration curves for amphiprotic species; determining the equivalence point; feasibility of acid- base titrations; magnitude of the equilibrium constant; effect of concentration; typical applications of acid-base titrations.

UNIT II: Precipitation and Redox Titrations **12 Hours**

Precipitation titrations- introduction; feasibility; titration curves- effect of reaction completeness, effect of titrant and analyte concentration, indicators for precipitation titrations; the Volhard, the Mohr and the Fajans methods; determining the equivalence point of mixture for anions; typical applications of standard silver nitrate solution.

Redox titration- introduction, electrode potentials in equilibrium systems; equilibrium constants and its calculation; detection of end point and redox indicators, choice of indicator, structural aspect of redox indicators, specific and nonspecific indicators; equivalence point determination from redox titration curves, derivatives of titration curves; formal redoxpotentials calculation; factors affecting the shape of titration curves- concentration; completeness of reaction; feasibility of redox titrations; sample preparation- pre-reduction and pre-oxidation; applications.

UNIT III: Complexometric Titrations **12 Hours**

Introduction; reactions of complex formation; stability of complexes; stepwise formationconstants; inorganic complexing agents- titrations involving unidentate ligands; titration of chloride with Hg^{2+} and cyanide with Ag^{+}; organic complexing agents- amino carboxylic acid titration; EDTA- acidic properties of EDTA; EDTA complexes with metal ions; equilibrium
calculations involving EDTA in solution; conditional formation constants; EDTA titration curves; determining the equivalence point; effect of other complexing agents on EDTA; factors affecting the titration curves; completeness of reaction; theory of common indicators; types of titration using

EDTA**,** selectivity, masking and demasking agents; applications of EDTA titrations- hardness of water; magnesium and aluminium in antacids; magnesium and zinc in a mixture; analysis of ores and foods.

TEXT BOOKS:

Fundamentals of Analytical Chemistry, D. A. Skoog, D. M. West, F. J. Holler, S. R. Crouch; 8th Edition

REFERENCE BOOKS:

1. Principles and Practice of Analytical Chemistry, F. W. Fifield, D. Kealy; Backwell Science Ltd., London
2. Vogel's Text Book of Quantitative Chemical Analysis; 6th Edition
3. Analytical Chemistry, G. D. Christian; 5th Edition, John Wiley, NY
4. Instrumental Methods of Chemical Analysis, H. Kaur; Pragati Prakashan
5. Quality in the Analytical Chemistry Laboratory, E. Prichard; John Wiley and Sons, NY
6. Quantitative Analysis, R. A. Day, A. L. Underwood; Prentice-Hall

WEB REFERENCES:

1. https://chem.libretexts.org/Bookshelves/Ancillary_Materials/Demos%2C_Techniques%2C_and_Experiments/General_Lab_Techniques/Titration/Acid-Base_Titrations
2. https://opentextbc.ca/chemistry/chapter/14-7-acid-base-titrations/
3. https://chem.libretexts.org/Courses/Northeastern_University/09%3A_Titrimetric_Methods/9.5%3A_Precipitation_Titrations
4. https://chem.libretexts.org/Bookshelves/General_Chemistry/Map%3A_Chemistry_-_The_Central_Science_(Brown_et_al.)/17%3A_Additional_Aspects_of_Aqueous_Equilibria/17.3%3A_Acid-Base_Titrations
5. https://chem.libretexts.org/Bookshelves/Analytical_Chemistry/Supplemental_Modules_(Analytical_Chemistry)/Quantifying_Nature/Volumetric_Chemical_Analysis_(Shiundu)/14.4%3A_Complex_ion_Equilibria_and_Complexometric_Titrations

Course Code: PGM-CHE-AC-C502
Course Title: Separation Techniques
Credits: 3
Duration: 36 Hours
Maximum Marks: 75

Course Objectives:

1. To give students a theoretical and practical introduction to the techniques of separation
2. To address modern challenges across the chemical, biological, and physical sciences as it is often necessary to isolate and examine chemical and biological species as pure substances

Course Outcomes:

On successful completion of the course, the student will be able to:

CO1: Describe the methods of separation and their applications

CO2: Acquire technical knowledge, practical experience with respect to chromatography and capillary electrophoresis

CO3: Understand various chromatographic techniques employed

CO4: Learn applications of various processes for separation and purification of compounds

UNIT I: Basic Separation Techniques and Electrophoresis methods 12 Hours

General aspects of separation techniques- role of separation techniques in analysis; classification; choice of separation method; distillation- theory, principle, apparatus; operation variables and their effect; relative volatility, reflux ratio, theoretical plates and HETP; distillation columns- types and choice; applications; molecular distillation- theory; setup and applications; sublimation-

theory, principle, apparatus, applications; centrifugation and ultracentrifugation- theory, principle and applications; Electrophoresis- introduction, types of electrophoresis techniques; instrumentation and theory of capillary electrophoresis, types of capillary electrophoretic methods- capillary zone electrophoresis, micellar electrokinetic capillary chromatography; Capillary Gel Electrophoresis; Capillary electrochromatography; applications.

UNIT II: Advanced Chromatographic Techniques 12 Hours

Introduction to theory and principle of chromatographic technique; terms and parametersused in chromatography, band broadening and column efficiency; variables that affect column efficiency; Van Deemter equation and its modification; Gas Chromatography- introduction, principle, theory, instrumentation; columns in GC; detectors- ionization, flame ionization, thermal conductivity, electron capture; evaluation of gas chromatogram; identification of chromatogram; applications; comparison of GSC and GLC; applications; High Performance Liquid Chromatography- introduction; principle; instrumentation; pumps, column and column packing; column efficiency and selectivity; characteristics of liquid chromatography; types of detectors- UV, RI, and fluorescence detectors; advantages, comparison of HPLC and GLC; applications; Numerical on chromatographic parameters.

UNIT III: Miscellaneous Separation Techniques and Hyphenated Techniques 12 Hours

Gel chromatography- introduction, theory; principle of gel permeation chromatography- instrumentation and applications; theory and mechanism of ion exclusion; applications of ion exclusion technique; inorganic molecular sieves; principle; types of sieves; applications. Supercritical Fluid Chromatography-introduction; theory, principle; properties of supercritical-fluids; instrumentation and operating variables; comparison of SFC and other column methods, applications; Field-flow fractionation- theory, mechanism, types and applications; Hyphenated Techniques- introduction; principle, instrumentation, applications of GC-FTIR; GC-MS; LC-MS, TG-MS.

TEXT BOOK:

Fundamentals of Analytical Chemistry, D. A. Skoog, D. M. West, F. J. Holler; 9th Edition

REFERENCE BOOKS:

1. Chemical Instrumentation: A Systematic Approach, H. A. Strobel
2. Analytical Chemistry, G. D. Christian; 5th Edition, John Wiley and Sons, NY
3. Instrumental Methods of Chemical Analysis, H. Kaur; Pragati Prakashan
4. Vogel's Text Book of Quantitative Chemical Analysis; 6th Edition
5. Instrumental Methods of Analysis, H. H. Willard, L. L. Merritt, J. A. Dean
6. Instrumental Methods of Chemical Analysis, B. K. Sharma; Goel Publishing House

WEB REFERENCES:

1. https://www.nottingham.ac.uk/-sczsteve/Ohlendieck%20and%20Harding%202018.pdf
2. http://www.chem1.com/acad/webtext/solut/solut-5.html
3. https://www.ijarnd.com/manuscripts/v2i4/V2I4-1168.pdf
4. https://www.pharmatutor.org/pharma-analysis/explain-electrophoresis-its-principle-and-factors-governing-it
5. https://www.iitk.ac.in/dordold/index.php?option=com_content&view=category&layout=blog&id=220&Itemid=239

Course Code: PGM-CHE-AC-C503
Course Title: Spectral Methods of Analysis
Credits: 3
Duration: 36 Hours
Maximum Marks: 75

Course Objectives:

1. To provide students the basics for the materials characterization by using XRD
2. To enable students to understand the concept of emission measurement for quantification of related compounds
3. To provide students the basic knowledge about the spectroscopy for identification of inorganic compounds

Course Outcomes:

On successful completion of the course, the student will be able to:

CO1: Understand the basics of emission and diffraction concepts

CO2: Understand the different phenomenon of emission

CO3: Understand the use of EDAX

CO4: Apply the knowledge of Mossbauer and electron spin spectroscopy in identification of compounds

UNIT I: X-ray Absorption, Neutron Diffraction Spectroscopy 12 Hours

A. X-ray absorption- introduction, theory, origin and interaction of X-ray with matter; X-ray spectrometer; Bragg's law; interpretation of X-ray diffraction pattern; calculation of lattice parameters; neutron diffraction- introduction, theory, instrumentation and applications; X-ray fluorescence- introduction, applications; X-ray photoelectron spectroscopy.

B. Theory and interpretation of micrographs by SEM, EDAX, TEM, AFM.

UNIT II: Molecular Fluorescence, Phosphorescence and Chemiluminescence 12 Hours

Fluorescence and phosphorescence- introduction, definition; principles of fluorescence, chemical structure and fluorescence; theory of molecular fluorescence; instrumentation- single and double beam filter fluorimeters; relationship between intensity of fluorescence and concentration; factors influencing fluorescence and phosphorescence; basic differences in fluorescence and phosphorescence measurement; advantages, limitations and precautions; spectrofluorometer; phosphorimeter; selection of excitation wavelength for analysis; reporting fluorescence spectra; applications of fluorimetric analysis- inorganic, pharmaceutical, agricultural, biochemical and biomedical materials; Chemiluminescence- introduction, principle, types; meaning of luminescence, chemiluminescence; instrumentation; chemiluminescence titrations, chemiluminescence measurement; quantitative chemiluminescence; gas phase chemiluminescence analysis; electro- chemiluminescence.

UNIT III: Mossbauer Spectroscopy and Raman Spectroscopy 12 Hours

Mossbauer Spectroscopy- introduction; principle; theory; instrumentation; line width; isomer shift; quadrupole interaction; magnetic interaction; information on spin and oxidation states; structure and bonding; spin transition from spectra of different Mossbauer active nuclei in various environments; Mossbauer effect; application of Mossbauer effect to investigate the compounds of iron and tin; Raman spectroscopy- introduction, light scattering by molecules, Raman effect- in solids, liquids, gases; mechanism; molecular structure; nature of Raman spectra; Raman activity of molecular vibrations; dynamic light scattering; determination of colloidal particle size.

TEXT BOOK:

Fundamentals of Molecular Spectroscopy, C. N. Banwell, E. M. McCash; 4th Edition, Tata McGraw-Hill, New Delhi

REFERENCE BOOKS:

1. Elements of X- ray Diffraction, B. D. Cullity; Addison Wisley
2. Diffraction Method, Wormald; Oxford University Press
3. Neutron Scattering in Chemistry, E. Butleworth Baun, G. London
4. Mossbauer Spectroscopy, N. N. Greenwood, T. C. Gibbs; Chapmann Hall
5. Chemical Application of Mossbauer Spectroscopy, V. I. Goldanski and R. H. Harber;

Academic Press
6. Spectroscopy in Inorganic Compounds, CNR Rao, G. R. Ferraro; Academic Press
7. Basic Principles of Spectroscopy, R. Cheney; Mc Graw-Hill
8. Principles of Instrumental Analysis, D. A. Skoog, F. J. Holler; 5th Edition
9. Instrumental Methods of Chemical Analysis, B. K. Sharma; Goel Publishing House

WEB REFERENCES:

1. https://serc.carleton.edu/research_education/geochemsheets/techniques/XRD.html
2. https://chem.libretexts.org/Bookshelves/Analytical_Chemistry/Map%3A_Principles_of_Instrumental_Analysis_(Skoog_et_al.)/15%3A_Molecular_Luminescence_Spectrometry
3. https://www.sciencedirect.com/topics/earth-and-planetary-sciences/mossbauer-spectroscopy
4. https://serc.carleton.edu/research_education/geochemsheets/techniques/mossbauer.html
5. https://www.google.com/url?sa=t&source=web&rct=j&url=https://www.nanoscience.com/techniques/atomic-force-microscopy/&ved=2ahUKEwjS-enSyJHnAhWXTX0KHWw1BqoQFjAaegQIAhAB&usg=AOvVaw2ou89f5fahKqUBqZgmLuIc&cshid=1579502355346.

VIDEO REFERENCES:

1. https://www.youtube.com/watch?v=5KLBrnauilg

Course Code: PGM-CHE-AC-C504
Course Title: Experiments in Analytical Chemistry
Credits: 3
Duration: 72 Hours
Maximum Marks: 100

Course Objectives:

1. To enable students in understanding the knowledge of separation and characterization
2. To enable students to carry out, record and analyze the result of analytical experiments

Course Outcomes:

On successful completion of the course, the student will be able to:
CO1: Understand the quantitative approach towards various instruments
CO2: Identify appropriate method to carry out quantitative analysis for desired samples
CO3: Perform titrimetric and spectrophotometric analysis
CO4: Develop good laboratory practices, both conceptually and practically

This course consists of seven units of experiments in various areas of Analytical Chemistry. Each Unit is equivalent to twelve hours duration. Any six units experiments to be performed.

UNIT I: Analysis of Pharmaceutical Tablets / Samples

1. Estimation of calcium from dietary supplements using Murexide indicator
2. Estimation of Ibuprofen / Paracetamol
3. Estimation of sulphadiazine / sulphonamide
4. Determination of neutralising power of tablets of different brands and compare effectiveness
5. Determination of iron using Zimmermann-Reinhardt reagent by titrating against potassium permanganate
6. Estimation of iron from given pharmaceutical drug sample using thioglycolic acid

UNIT II: Ion Exchange Chromatography and Solvent Extraction Method

1. To determine the capacity of a cation exchange resin
2. To determine the capacity of an anion exchange resin
3. To determine the Fe ion as Fe-oxine complex using Butyl acetate/ $CHCl_3$ as extracting solvent

4. To separate the acidic, basic and neutral compounds from the mixture by solvent extraction

UNIT III: Electrochemical Method

1. pH-metric determination of hydrolysis constant of aniline hydrochloride
2. pH-metric determination of the acid-base dissociation constant and isoelectric point of amino acid
3. pH metric determination of dissociation constant of dibasic, oxalic acid
4. Potentiometric estimation of carbonate and bicarbonate from the mixture
5. Potentiometric determination of dissociation constant for Cu-ammonia complex
6. To determine the critical micelle concentration of the detergent using conductometer

UNIT IV: Gas and HPLC Chromatographic Analysis

1. Optimum flow rate for the determination of chloroform using Van Deemter equation
2. Quantitative analysis of a mixture of chloroform and carbon tetrachloride
3. Gas chromatographic analysis for a mixture of gases like O_2, N_2 and CO_2
4. Analysis of mixture of alcohols using HPLC
5. To study the quantitative assay of ampicillin injection powder by using HPLC
6. To analyze the mixture of two hydrocarbons (Toluene and Nitrobenzene) by HPLC
7. Analysis of Ibuprofen/Paracetamol (analgesics) in a commercial sample/tablet byHPLC
8. To develop and validate the analytical method of any one drug using GC/HPLC
9. To determine the number of theoretical plates by HPLC using Acetophenone asreference material

UNIT V: Simple Chromatography

1. To separate alpha amino acids by paper chromatography
2. To separate the two organic compounds from the mixture by TLC
3. To separate the leaf pigments: chlorophyll 'a' chlorophyll 'b', carotene and xanthophylls by paper chromatography
4. To determine the R_f value of glycine by ascending paper chromatography
5. To separate sugars and amino acids by paper and thin layer chromatography
6. To separate the mixture of o- and p- nitro anilines by column chromatography
7. To study the presence of lactose in milk by descending paper chromatography

UNIT VI: Spectrophotometric Method

1. To determine pka value of methyl red indicator at room temperature
2. To determine the indicator constant and isobestic point of an indicator
3. To determine the stoichiometry and stability constant of ferric salicylic acid complexby Job`s method and mole ratio method
4. To determine the amount of each p-nitrophenol and m-nitrophenol from the mixtureby spectrophotometric titration using standard NaOH solution at λ_{max}= 280 nm
5. To record the UV absorption spectrum of acetone in n-hexane and identify the various transitions
6. To estimate the amount of aspirin and caffeine from APC tablet by UV-Visible spectrophotometry
7. To study the iodination of acetone by spectrophotometric method
8. To estimate the amount of arsenic in dried shrimp by UV-Visible spectrophotometry using molybdenum blue method.
9. To estimate Pb/Hg by AAS method

UNIT VII: Interpretation Exercise

1. X-ray powder diffraction analysis of cubic compound:
    a. Determination of Lattice constants and crystallite Size
    b. Density

2. Interpretation of Mossbauer spectrum with reference to determination of: isomer shift; quadruple splitting; internal magnetic field; general comment
3. Interpretation of IR spectrum with reference to stretching vibration of: C=N; C=O; N-O; M-O
4. Interpretation of NMR spectrum with reference to calculation of chemical shifts and general comments
5. Interpretation of absorption spectra for:
    a. Verification of the position of ligands in spectrochemical series
    b. Calculation of spectral splitting parameters
    c. Determination of geometry of a given compound (octahedral, tetrahedral, square planar)
6. Statistical revaluation of spectrophotometric data

REFERENCE BOOKS:

1. Vogel's Textbook of Quantitative Chemical Analysis, 6th Edition
2. Comprehensive Experimental Chemistry, V. K. Ahluwalia; New Age Publications
3. Experimental Physical Chemistry, F. Daniels and J. Williams
4. Experimental Physical Chemistry, R. C. Das and B. Behera
5. Practical Physical Chemistry, B. Viswanathan, P. S. Raghavan
6. An Introduction to Practical Biochemistry, D. T. Plummer; 3rd Edition, Tata Mc Graw-Hill, New Delhi
7. Advanced Physical Chemistry, J. B. Yadav; 14th Edition, Goel Publishing House
8. Systematic Experimental Physical Chemistry, S. W. Rajbhoj, T. K. Chondhekar; Anjali Publication, Aurangabad.

VIDEO REFERENCES:

1. https://www.youtube.com/watch?v=lha8dEBNFS4&t=251s

ELECTIVE COURSES

Course Code: PGM-CHE-AO-E501
Course Title: Advanced Mass Spectrometry
Credits: 2
Duration: 24 Hours
Maximum Marks: 50

Course Objectives:

1. To enable students to understand the basics of Mass spectrometry, different ionisation methods, mass analysers and its application to solve structural problems of proteins

Course Outcome:

On successful completion of the course, the student will be able to:
CO1: Choose a proper technique for the analysis of the desired compound
CO2: Interpret and recognise various mass spectra
CO3: Solve and elucidate structures of various organic compounds
CO4: Explain and understand various ionisation processes and recognise different spectrabased on ionisation modes.

UNIT I: Ionisation Sources **12 Hours**

Mass Spectrometry- introduction, principle, instrumentation of mass spectrometer; electron ionization; chemical ionization; proton transfer; adduct formation; charge-transfer chemical ionization; reagent gas; negative ion formation; desorption chemical ionization; field ionization; field desorption; fast atom bombardment and liquid secondary ion mass spectrometry; field

desorption; plasma desorption; laser desorption; matrix-assisted laser desorption ionization MALDI; thermo spray; atmospheric pressure ionization, atmospheric pressure- photo ionization; electro spray ionization; thermal ionization source; spark source; glow discharge source; inductively coupled plasma source.

UNIT II: Mass Analysers and Applications of MS **12 Hours**

Quadrupole analysers; ion guide and collision cell; MS^n, time-of-flight analysers; linear time-of-flight mass spectrometer; delayed pulsed extraction; reflectrons; tandem mass spectrometry with time-of-flight analyser; magnetic and electromagnetic analysers; tandem mass spectrometry in electromagnetic analysers; fragmentation reactions; tandem massanalysis, proteomics.

TEXT BOOK:

Mass Spectrometry: Principles and application, Edmond D. Hoffmann; Vincent Stroobant John Wiley

REFERENCE BOOKS:

1. Mass Spectrometry: A Textbook, Jurgen H. Gross; 2nd Edition, Springer
2. Electrospray and MALDI Mass Spectrometry: Fundamental, Instrumentations and Practicalities and Biological Applications, Richard B. Cole; John Wiley

WEB REFERENCES:

1. http://chemistry.emory.edu/msc/tutorial/mass-spectrometry-ionization.html
2. http://chemguide.co.uk/analysis/masspec/fragment.html
3. https://chem.libretexts.org/Bookshelves/Organic_Chemistry/Map%3A_Organic_Chemi (Wade)/11%3A_Infrared_Spectroscopy_and_Mass_Spectrometry/11.08%3A_Fragmentation _Patterns_in_Mass_Spectrometry
4. https://chem.libretexts.org/Bookshelves/Analytical_Chemistry/Supplemental_Modules_(An alytical_Chemistry)/Instrumental_Analysis/Mass_Spectrometry/Mass_Spectrometers_(Instru mentation)/Mass_Analyzers_(Mass_Spectrometry)
5. Schwartz J C, Senko M W, Syka J E P. A two-dimensional quadrupole ion trap mass spectrometer. Journal of the American Society for Mass Spectrometry, 2002, 13(6): 659-669

Course Code: PGM-CHE-AO-E502
Course Title: Advanced NMR Spectroscopy
Credits: 2
Duration: 24 Hours
Maximum Marks: 50

Course Objectives:

1. To enable students to understand basic aspects of nuclear magnetic resonance spectroscopy
2. To enable students to understand one-dimensional NMR, Chemical shifts, J-coupling, Interpretation of 1D NMR spectrum, basics of 2D NMR, different 2D NMR experiments and their application/interpretation

Course Outcomes:

On successful completion of the course, the student will be able to:
CO1: Explain the concept of nuclear magnetic resonance spectroscopy
CO2: Apply nuclear magnetic resonance spectroscopy for identifying organic compound
CO3: Explain the concept of 2D NMR spectroscopy
CO4: Apply 2D NMR to identify organic compounds

UNIT I: NMR and ^{13}C-NMR Spectroscopy **12 Hours**

Nuclear magnetic resonance- theory, quantum description; classical description of NMR; types of

NMR spectra; applications of proton NMR in qualitative and quantitative analysis (in general); CW and PFT techniques; Types of CMR spectra-undecoupled- proton decoupled-off-resonance decoupled (SFORD)-selectivity decoupled and gated ^{13}CJ) and heteronuclear (^{13}C-^{1}H, ^{13}C-^{2}HJ) couplings, nuclear overhauser effect, ATP (attached proton test), DEPT

UNIT II: 2D-NMR Spectroscopy **12 Hours**

Classification of 2D experiments- 2DJ resolved spectroscopy- HOMO and HETERO- 2DJ Resolved Spectra: correlation spectroscopy (COSY) - HOMO-COSY, 2D-INADEQUATE and NOESY.

TEXT BOOK:

Spectroscopic Identification of Organic Compounds, R. M. Silverstein, G. C. Bassler and T. M. Morril

REFERENCE BOOKS:

1. Spectroscopic Identification of Organic Compounds, R. M. Silverstein and Webster
2. NMR in Chemistry- A Multinuclear Introduction, William Kemp
3. ^{13}C NMR for Organic Chemists, G. C. Levy, G. L. Nelson
4. Understanding NMR Spectroscopy, James Keeler; 2nd Edition

WEB REFERENCES:

1. http://chem.ch.huji.ac.il/nmr/techniques/2d/2d.html
2. http://www.cryst.bbk.ac.uk/PPS2/projects/schirra/html/2dnmr.htm
3. http://chem.ch.huji.ac.il/nmr/techniques/2d/cosy/cosy.html
4. http://www-keeler.ch.cam.ac.uk/lectures/2d_a4.pdf
5. http://chem.ch.huji.ac.il/nmr/techniques/2d/noesy/noesy.html

Course Code: PGM-CHE-AO-E503
Course Title: Applied Analytical Chemistry
Credits: 2
Duration: 24 Hours
Maximum Marks: 50

Course Objectives:

1. To enable students with a knowledge of various methods for identification of compounds using spectroscopy and to determine the quantitative analysis of sample
2. To enable students to analyse various constituents in compounds in various fields like clinical chemistry and cosmetics analysis

Course Outcomes:

On successful completion of the course, the student will be able to:
CO1: Understand the basic concepts used in clinical chemistry
CO2: Understand the chemistry of food and will be able to analyse different components in it
CO3: Get an idea about the nutritional values of food stuff
CO4: Apply the knowledge of analytical chemistry for analysing cosmetics

UNIT I: Food Analysis, Processing and Preservation **12 Hours**

Food legislation and public health; nutritional value of foods; general methods for determination of moisture, ash, crude protein, fat, crude fibre, carbohydrates; analysis of foodand beverages (soft drinks, alcoholic drinks)-calcium, potassium, sodium and phosphates; edible oils and fats- general composition of edible oils; detection of purity; test for common edible oils; rancidity of fats and oils; estimation of rancidity; determination of ratio between saturated and unsaturated fatty acids; determination of- total fatty acid, acid value, iodine value, ester value, acetyl value, titre value, peroxide value, R. M. value, P.V. value.

Food processing and preservation-introduction; food processing; food preservation methods-freezing, drying, pasteurization, sterilization, irradiation, canning, concentration; analysis of preservatives; types of packing materials and properties; industrial requirements.

UNIT II: Clinical Chemistry and Cosmetics Analysis 12 Hours

A. Clinical Chemistry- introduction; sample collection and preservation of physiological fluids; composition of body fluid; detection of abnormal levels of certain constituents leading to diagnosis of diseases; analysis of physiological fluids like- blood, urine, serum; estimation of blood glucose, cholesterol, urea, haemoglobin, billirubin, uric acid, urea in urine, calcium, phosphate; physiological and nutritional significance of water soluble and fat-soluble vitamins, minerals.

B. Cosmetics analysis- introduction, analysis of lipsticks- determination of non-volatile matter, lakes and fillers; analysis of deodorants and antiperspirants for- Al, Zn, boric acid, chloride, sulphate, urea; analysis of face powder- fats, fatty acid, Ca, Mg, $BaSO_4$, Ti and Fe; oxides of Ti, Fe and Al (total); analysis of hair tonic: 2, 5- diamino toluene, $KBrO_3$, resorcinol, salicylic acid.

TEXT BOOK:

Food Composition and Analysis, H. O. Triebold, L. W. Aurand

REFERENCE BOOKS:

1. Introduction to Food Science and Technology Series, G. F. Stewart, M. A. America; Academic Press
2. Food Chemistry, H. K. Chopra, P. S. Panesar; Narosa Publication
3. Food Chemistry; Alex V. Ramani; M. J. P. Publishers
4. Analytical Chemistry of Foods, Ceiwyn S. James; 1st Edition, Blackie Academic and Professional Chapman and Hill Publisher
5. Chemical Analysis of Food, Pearson
6. Practical Biochemistry in Clinical Medicine, R. L. Nath; 2nd Edition, AcademicPublishers
7. Analytical Biochemistry, D. J. Holme, H. Peck; Longman
8. Bio analytical Chemistry, S. R. Mikkelsen, E. Corton; John Wiley and Sons
9. Chemical Analysis of Food and Food Products, H. B. Jacob; Van Westrand Reinhold

WEB REFERENCES:

1. https://www.news-medical.net/life-sciences/Clinical-Chemistry-Tests.aspx
2. https://www.sciencedirect.com/science/article/pii/0379073881901730
3. https://www.slideshare.net/mobile/parth241989/analysis-of-cosmetics-112070804018
4. https://www.sciencedirect.com/science/article/pii/S2214750015000165
5. https://sciencemonk.com/forensic-chemistry/

Course Code: PGM-CHE-AO-E504
Course Title: Bio analytical Chemistry
Credits: 2
Duration: 24 Hours
Maximum Marks: 50

Course Objectives:

1. To enable students to the techniques routinely used in bio analytical laboratories
2. To enable students to study various bio analytical techniques used for diagnosis of diseases

Course Outcome:

On successful completion of the course, the student will be able to:CO1: Have valuable training in forensic science and biotechnology
CO2: Understand antibody-antigen interactions
CO3: Understand various bio analytical techniques used for medical diagnosis and research

CO4: Understand the working of various biosensors used to detect biological compounds

UNIT I: Antibodies, spectroscopic methods for matrix characterization 12 Hours

Antibodies- Introduction, structural, functional properties of antibodies, polyclonal and monoclonal antibodies; antibody- antigen interactions; analytical applications of secondary antibody-antigen interactions: agglutination reactions and precipitation reactions; keys to immunochemical measurements; analytical applications of biological tracers; principle and applications of radioimmunoassay (RIA); enzyme linked immune sorbent assay (ELISA); Introduction to the concept of RTPCR; immuno histochemistry- important diagnostic tool; introduction to protein; method for total protein- Lowry, Smith, Bradford; protein quantification methods; methods for total DNA- fluorometric, diphenylamine; total RNA; determination of total carbohydrate- ferricyanide, phenol sulphuric acid; Purpald assay for bacterial polysaccharides; free fatty acids.

UNIT II: Biosensors and Bio analytical approaches 12 Hours

Introduction to biosensors; examples of biosensor; configurations; response of enzyme-based biosensors; ferrocene-mediated amperometric glucose sensor; potentiometric biosensor for phenyl acetate; potentiometric immune sensor for digoxin; evanescent-wave fluorescence biosensor for bungaro toxin; optical biosensor for glucose based on fluorescence energy transfer; piezoelectric sensor for nucleic acid detection, enzyme thermistors; clinical genomics; proteomics and metabolomics; clinical diagnosis and screening; research and development; emerging pharmaceutical products, future perspectives; structure and characteristics of key transition metals, importance of transition metals in physiological processes, transition metals as mediators of disease processes, therapeutic implications of transition metals, determination of transition metals in nature.

TEXT BOOK:

Understanding Bio analytical Chemistry, V. A. Gault; John-Wiley and Sons

REFERENCE BOOK:

1. Analytical Biochemistry, D. J. Holme; Pearson Education Ltd.
2. The Principels of ion-selective electrodes and membrane transport, W. E. Morf
3. Bio analytical Chemistry, S. R. Mikkelsen; John-Wiley and Sons

WEB REFERENCES:

1. https://www.elprocus.com/what-is-a-biosensor-types-of-biosensors-and-applications/
2. Mehrotra, P. (2016, January 6). Biosensors and their applications – A review. Journal ofOral Biology and Craniofacial Research. doi:10.1016/j.jobcr.2015.12.002
3. https://www.radiologyinfo.org/en/info.cfm?pg=bodymr
4. https://www.iaea.org/topics/radiotracers
5. https://www.antibodies-online.com/resources/17/1215/radioimmunoassay-ria/

Course Code: PGM-CHE-AO-E505
Course Title: Calibrations and Validation
Credits: 2
Duration: 24 Hours
Maximum Marks: 50

Course Objectives:

1. To enable students to understand the validation characteristics of some procedures used in laboratory
2. To enable students to have an idea about ICH guidelines used in pharmaceutical industry

Course Outcomes:

On successful completion of the course, the student will be able to:

CO1: Understand the qualification of laboratory equipment as a precondition of reliableanalytical testing

CO2: Understand the basic rules of documentation in QA

CO3: Calibrate the instruments of industrial importance

CO4: Have the knowledge of ICH guidelines in method development

UNIT I: Regulations and Qualifications **12 Hours**

Regulations: Regulatory requirements for analytical method validation; validation of analytical methods; complete method validation package, analytical data, protocol, plan, revisions and change controls; International Conference on Harmonization (ICH) Guideline Q2A: Validation of analytical procedures; linearity and range criteria and their role in instrumental method validation; GMP (US), Qualification: Overview of qualification of instruments; installation, operation and performance qualification (IQ, OQ, PQ) of analytical equipments; method validation for UV-Visible Spectrophotometer, IR Spectrophotometer, Spectrofluorometer, HPTLC, GC, HPLC; qualitative and quantitative method validation; parameters of validation; statistics in validation; detailed discussion on accuracy and precision role in method validation; protocols and interpretation.

UNIT II: Calibration **12 Hours**

Calibration of analytical balance and pH meter; role of quantification limit and specificity; Limit of Detection (LOD) and Limit of Quantification (LOQ); Robustness and method validation; Ruggedness of chromatographic method; Ruggedness of sample preparation procedure; Calibration verses Qualification verses Validation; Case study for HPLC, UV; calibration of various instruments used for drug analysis like HPTLC, UV-Visible Spectrophotometer, IR Spectrophotometer, Spectro fluorimeter, GC, HPLC.

REFERENCE BOOKS:

1. The Theory and Practice of Industrial Pharmacy Lachman Edition
2. Web Resources in Pharmacy, In Pharma Publication, Bangalore
3. Schedule M
4. WHO Guideline
5. Analytical Method Development and Validation, Michael E. Swartz
6. Pharmaceutical Process Validation, Loftus and Nash
7. Vogel's Textbook of Quantitative Chemical Analysis, J. Mendham, R. C. Denny, J. D. Banes, Thomas; 6th Edition, ELBS
8. Pharmaceutical Process Validation, Alfred H. Wachter
9. Validation and Qualification in Analytical Laboratories, Ludwig Huber; 2nd Edition, Wiley Publisher

WEB REFERENCE:

1. https://uc.xyz/1mhmZR?pub=link
2. https://www.researchgate.net/publication/8508200_Qualification_of_analytical_instruments_for_use_in_the_pharmaceutical_industry_A_scientific_approach/link/02bfe50f872c59f953000000/download
3. https://www.slideshare.net/mobile/dhavalrock24/concept-of-ursdqiqoqpq
4. https://www.ncbi.nlm.nih.gov/pmc/articles/PMC4670047/
5. https://www.pharmaguideline.com/2010/05/calibration-of-uv-visible.html?m=1
6. https://nvlpubs.nist.gov

Course Code: PGM-CHE-AO-E506
Course Title: Chemometrics
Credits: 2
Duration: 24 Hours
Maximum Marks: 50

Course Objectives:
To provide students with a basic tool in solving problems

Course Outcomes:
On successful completion of the course, the student will be able to:
CO1: Handle computers and data sheet
CO2: Handle statistical arrangements of data

UNIT I: Introduction to Data and Statistics **12 Hours**
Introduction; univariate statistics review; probability; variance and sampling, linear regression and calibration data, digitization, and the Nyquist Theorem, detection limit, S/N ratio, and signal filtering; review of linear algebra: scalars, vectors, and matrices, matrix notation and matrix operations orthogonality, analysis of variance (ANOVA)- 1 variable, analysis of variance- 2 variables; introduction to Matlab^{TM}: programmed, basics and layout, matrix operations in Matlab^{TM} the diary command and examples, ANOVA in Matlab^{TM} experimental design: factorial design, simple versus complex models, factorial design in Matlab^{TM}; half-factorial design.

UNIT II: Multivariate Methods **12 Hours**
A. Introduction to various multivariate methods; the six habits of a chemometrician; principle component analysis (PCA); data pretreatment- mean centering and normalization; PCA in Matlab^{TM}.
B. Classical least squares (CLS), CLS in Matlab^{TM}, inverse least squares (ILS).
C. Multiple linear regression (MLR); principle component regression (PCR); partial least squares, examples in Matlab^{TM}; summary of multivariate methods; pattern recognition- supervised versus unsupervised pattern recognition, K nearest neighbours (KNN); soft independent modelling for chemical analysis (SIMCA), summary of pattern recognition.

TEXT BOOK:
Chemometrics, A Practical Guide; Kenneth R. Beebe, Randy J. Pell, and Mary BethSeasholtz, John Wiley and Sons, Inc., New York

REFERENCE BOOK:
The computer program MATLAB^{TM} will be required for some portions of the course

Course Code: PGM-CHE-AO-E507
Course Title: Techniques in Chemical Analysis
Credits: 2
Duration: 24 Hours
Maximum Marks: 50

Course Objectives:
1. To illustrate to students the basic principles of modern instrumental methods
2. To enable students in understanding the basic theory underlying the construction of several common instruments and to become familiar with the operation of spectroscopic as well asnon-spectroscopic techniques

Course Outcomes:
On successful completion of the course, the student will be able to:
CO1: Develop an understanding of the range and theories of instrumental methods available in

analytical chemistry

CO2: Have theoretical knowledge on selected instrumental methods of analysis

CO3: Have the knowledge on analytical study by spectroscopy

CO4: Understand and compare a range of analytical techniques and explain the underlying principles

UNIT I: Spectrophotometric, Nephelometry and Turbidimetry Analysis 12 Hours

Spectrophotometry- introduction; law of absorption; absorbance and transmittance spectrum; technique for colour comparison; radiation sources; wavelength selection; standard cells; photo detectors; spectrophotometer instrumentation- single and double beam spectrophotometer; presentation of spectral data; spectrophotometric titrations; applications- determination of Mn (II), Fe (III) as thiocyanate, Cu (II) using salicyladoxime, simultaneous determination of Mn (II) and Cr (VI).

Turbidimetry- introduction; principle; instrumentation; concentration effects; particle size and wavelength on scattering; turbidimetric titrations; applications.

Nephelometry- introduction; principle; instrumentation; concentration effects; particle size and wavelength on scattering; choice between the nephelometry and turbidimetry, turbidimetry and colorimetry, nephelometry and fluorimetry; applications.

UNIT II: Refractometry and Polarimetry 12 Hours

Refractometry- introduction; theory and measurement of refractive index, factors affecting refractive index; instrumentation; types of refractometers; molecular refractivity and chemical constitution; applications of refractometry- qualitative and quantitative analysis; plain curves; cotton effect curves.

Polarimetry- introduction, theory, principle; plane polarized light; optical activity; theory of optical activity; applications of optical activity; instrumentation; application of optical rotation method in rate constant determination; acid- inversion of cane sugar; relative strengths of acids; optical rotatory dispersion and Circular Dichroism and its applications; selection rules; deduction of absolute configuration of molecules; octant rule for ketones and cotton effect.

REFERENCE BOOKS:

1. Textbook of Quantitative Inorganic Analysis, A. I. Vogel, Longman
2. Instrumental Methods of Chemical Analysis, G. W. Ewing, McGraw-Hill
3. Basic Concepts of Analytical Chemistry, S. M. Khopkar
4. The Principals of ion-selective electrodes and membrane transport, W. E. Morf
5. Analytical Chemistry, G. D. Christian; 5th Edition, John Wiley and Sons, NY
6. Instrumental Methods of Chemical Analysis, H. Kaur, Pragati Prakashan
7. Instrumental Methods of Chemical Analysis, B. K. Sharma; Goel Publishing House

WEB REFERENCES:

1. http://rxpharmaworld.blogspot.com/2016/12/nephelometry-and-turbidimetry.html
2. http://www.environmentalpollution.in/pollution/regulation- andmonitoring/nephelometry-and-turbidimetry-principle-theory-and-techniques/1880
3. https://www.microscopyu.com/techniques/polarizedlight/introduction-to-polarized-light

Course Code: PGM-CHE-AO-E508
Course Title: Thermal Methods of Analysis
Credits: 2
Duration: 24 Hours
Maximum Marks: 50

Course Objectives:

1. To provide students with knowledge of thermal analysis to enable them to understand the principle of operation.

2. Obtaining basic knowledge on thermoanalytical methods
3. Application of thermoanalytical instruments in practice

Course Outcomes:

On successful completion of the course, the student will be able to:

CO1: Choose the experimental conditions for the measurements and combine different thermoanalytical techniques

CO2: Analyze and present the results of the measurements.

CO3: Understand the principles of thermoanalytical techniques and combine different thermoanalytical techniques

CO4: Apply theoretical knowledge for practical analysis CO5: Analyse and present the results of the measurements

UNIT I: Thermogravimetric Analysis and Differential Thermal Analysis 12 Hours

Thermogravimetric Analysis- introduction; definition; instrumentation (all components to be discussed); information from TGA curve; factors affecting TGA curves- instrumental, characteristics of sample; advantages and limitation of TGA; calculation of compound composition, percent decomposition; applications of thermogravimetry; Derivative Thermogravimetry (DTG)- definition, comparison between TG and DTG.

Differential Thermal Analysis- introduction, definition; theoretical basis of DTA; DTA instrumentation (all components to be discussed); factors affecting the DTA curve; advantagesand disadvantages of DTA; applications of DTA.

UNIT II: Differential Scanning Calorimetry and Thermometric Titrations 12 Hours

Differential Scanning Calorimetry- definition; instrumentation of DSC, types, factors affecting DSC curves; comparison between DTA and DSC techniques; applications.

Thermometric Titrations- introduction; definition; instrumentation (all components to be discuss); Numerical based on TGA and DTA curves to calculate percent loss and fix the formula of the sample are to be solved.

TEXT BOOK:

Fundamentals of Analytical Chemistry, D. A. Skoog, D. M. West, F. J. Holler, S. R. Crouch; 8th Edition

REFERENCE BOOKS:

1. Principles and Practice of Analytical Chemistry, F. W. Fifield, D. Kealy; Backwell Science Ltd., London
2. Vogel's Textbook of Quantitative Chemical Analysis; 6th Edition
3. Analytical Chemistry, G. D. Christian; 5th Edition, John Wiley, NY
4. Instrumental Methods of Chemical Analysis, H. Kaur; Pragati Prakashan
5. Instrumental Methods of Chemical Analysis, Chatwal and Anand, Himalaya Publishing House

WEB REFERENCES:

1. https://www.currenta.com/analytics/methods/thermoanalytical-methods.html
2. http://web.abo.fi/instut/biofuelsGS-2/kursen/%C5A/lectures/Lectrure_Thermal%20Analysis.pdf
3. https://www.chemie-biologie.uni-siegen.de/ac/be/lehre/ss11/uebungen-solidstate/summary_of_tg_and_dta.pdf
4. https://www.pslc.ws/macrog/dsc.htm
5. https://www.brainkart.com/article/Thermometric-Titrations-(TT)_30858/

Course Code: PGM-CHE-AO-E509
Course Title: Quality Assurance and Quality Control in Analytical Chemistry
Credits: 2
Duration: 24 Hours
Maximum Marks: 50

Course Objectives:

1. To enable students to understand the basics of quality control and quality assurance
2. To enable students to describe the types of packaging and regulatory aspects in food and pharmaceutical industries

Course Outcomes:

On successful completion of the course, the student will be able to:
CO1: Explain the basics of quality assurance and quality control
CO2: Know the types of packaging and regulatory aspects in food and pharmaceuticalindustries
CO3: Handle reagents and chemicals appropriately
CO4: Evaluate the quality assurance data

UNIT I: Introduction to Quality Assurance and Quality Control 12 Hours

Introduction to basic concepts, quality assurance; aspect of specification and tolerance; quality acceptance; sampling reality; cost aspect of quality decisions; quality control in raw materials; finished product; laws related to quality control; case studies of quality control in various industries like pharmaceuticals, agrochemicals, petrochemicals, dyes, plastics, polymers; safety in laboratory; importance of laboratory note book; cleaning and marking laboratory ware; measuring volume; calibrating volumetric flask; selecting and handling reagents and chemicals; methods of quality assessment- internal and external; evaluating quality assurance data- prescriptive approach and performance based approach.

UNIT II: Standard Method, Analysis; Packaging and Regulatory Aspects 12 Hours

A. Development of a standard method and analysis- introduction; optimising experimental procedure (Standard Operating Procedures); verifying the method- single-operator characteristics; blind analysis of standard samples; ruggedness testing; validating standard method; two-sample collaborative testing and analysis of variance.

B. Packaging and Regulatory Aspects- introduction; types of packing material and regulations; acts in food and pharmaceutical industries; testing of material for packing; legal aspects in packing; regulatory aspects of foods, drugs and cosmetics; food safety and Standards Act, 2006; I.S.I., AGMARK, other standards for foods and cosmetics with reference to testing of foods, drugs and cosmetics; raw material testing; Government authorities concerned with testing- their qualification, duties, powers, procedure to follow; records to be maintained under the Acts; C.G.M.P. and C.G.L.P.S.; Department of WHO certification.

TEXT BOOK:

Fundamentals of Analytical Chemistry, D. A. Skoog, D. M. West, F. J. Holler, S. R. Crouch; 8th Edition

REFERENCE BOOKS:

1. Quality Assurance in Analytical Chemistry, W. Funk, V. Dammann, G. Donnevert; VCH Weinheim
2. Principles and Practice of Analytical Chemistry, F. W. Fifield, D. Kealy; Backwell Science Ltd. London
3. Vogel's Textbook of Quantitative Chemical Analysis; 6th Edition
4. Modern Analytical Chemistry, D. Harvey; McGraw-Hill Education
5. Analytical Chemistry, G. D. Christian; 5th Edition, John Wiley and Sons, NY
6. Instrumental Methods of Chemical Analysis, H. Kaur; Pragati Prakashan

7. Pharmacopeia of India, Volume I and II
8. Quality in the Analytical Chemistry Laboratory, E. Prichard; John Wiley
9. Principals of Package Development, Gribbinetal
10. Modern Packaging Encyclopaedia and Planning Guide- MacqraWreyco
11. Government of India Publications of Food Drug Cosmetic Acts and Rules

WEB REFERENCES:

1. https://asq.org/quality-resources/quality-assurance-vs-control
2. https://nvlpubs.nist.gov/nistpubs/Legacy/IR/nbsir85-3105.pdf
3. https://www.who.int/water_sanitation_health/resourcesquality/wqmchap9.pdf
4. https://www.who.int/medicines/areas/quality_safety/quality_assurance/control/en/
5. https://www.who.int/tdr/publications/documents/glp-handbook.pdf

NOTE: Students can opt either PGM-CHE-AO-D508: Dissertation; or PGM-CHE-AO-M 509: Modules in Experimental Chemistry and PGM-CHE-AO-I510: Internship Modules; both courses together.

PGM-CHE-AO-D510: DISSERTATION 196 Hours

The dissertation must comprise of original research and may be conducted either at the Institute or with approval, in an outside institution or company e. g., the student's employers. The guiding teacher may serve some laboratory hours for industry work.

The dissertation work is to be submitted for: evaluation and Viva Voice examination at the end of Semester IV.

Written test must be conducted regarding the basic principles of techniques or instruments used with respect to the area of dissertation topic.

Students may be assessed based on designing the question bank by students on dissertation topic.

PGM-CHE-AO-M 511: MODULES IN EXPERIMENTAL CHEMISTRY 96 Hours

There are Seven Modules on experiments of various areas of Chemistry. Each Module is equivalent to eight hours duration per week.

INSTRUMENTATION

MODULE I: IR SPECTROSCOPY

1. Quantification of acetyl group from polymers using IR
2. Plasticizer from PVC using IR
3. Determination of ethanol in gasoline
4. Spectral analysis of different compounds (synthesised inorganic complexes and organic compounds)
5. Following micro scale reaction using FTIR

MODULE II: POTENTIOMETRY

1. Potentiometric determination of reducing sugars
2. Potentiometric titration using graphite sensor
3. Kinetics of bromination reaction: A potentiometric study
4. Non-aqueous titration containing mixture of aniline and ethanolamine

MODULE III: GAS CHROMATOGRAPHY

1. Plasticizer from PVC using GC
2. Synthesis of high boiling organic compound by derivatisation and analyses by GC
3. Separation of alcoholic mixtures
4. Determination of alcoholic content in: i. Beer ii. Wine iii. Local drinks
5. Gas chromatographic analysis for: i. automobile exhaust ii. Cigarette smoke
6. Analysis of preservatives from solid and liquid samples (extraction, sample preparation and analysis)

MODULE IV: HPLC

1. Determination of caffeine content in: i. Tea ii. Coffee iii. Soft drinks iv. Chocolates
2. Qualitative and quantitative analysis of pharmaceutical Drug (e. g. aspirin)
3. Purity of the solvents using HPLC

MODULE V: TG/DTA/DSC

1. Determination of the purity of pharmaceuticals samples
2. Thermal properties of peanut proteins
3. Glass transition temperature of polymers (polymer to be used in preparation of membrane sensor)
4. Determination of water of crystallization in coordination compounds/ inorganic salts
5. Studies on thermal decomposition of Zinc NTA salt
6. DSC study on pharmaceutical product

MODULE VI: UV-VISIBLE SPECTROSCOPY

1. Method development and validation for a drug by UV/Visible spectrophotometer
2. Photometer (to build a photometer using LED) a guided-inquiry experiment to introduce analytical instrument
3. Determination of the composition of Ni and Fe (III) in a solution by spectrophotometric titration using Disodium salt of EDTA

MODULE VII: ATOMIC ABSORTION SPECTROSCOPY

1. Analysis of Na, K and Ca in water samples
2. Analysis of metal ion from soil /ore
3. Analysis of metal ion from alloys: Fe and Cr from steel / Zn from Brass / Sn andPb from solder
4. Analysis of Lead and cadmium in toys

MODULE VIII: NON-INSTRUMENTATION

1. Synthesis of nano composites
2. Analysis of Fats and oils- saponification value, iodine value, peroxide value, acid value
3. Determination of the rancidity of oil samples
4. Determination of acetic acid in vinegar
5. Synthesis of:
   i. Polystyrene using suspension polymerisation
   ii. Biginelli reaction (Solvent free synthesis)
   iii. Hydrogenation using Pd-C
   iv. Extraction of natural products using Soxhlet apparatus
6. Determination of copper in brass by complexometric method

PGM-CHE-AO-I512: INTERNSHIP MODULES **96 Hours**

MODULE A: Internship at Industry; One week per Semester (Semester III and IV) **72 Hours**

MODULE B: Write up of the Internship work per Semester (Semester III and IV) **08 Hours**

MODULE C: Students to design two modules based on their experience at industry **16 Hours**

*__Assessment to be done at the end of Semester IV__

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