List of Courses Focus on Employability/ Entrepreneurship/ Skill Development

Department : *Chemistry*

Programme Name : *M. Sc.*

Academic Year : 2017-18

List of Courses Focus on Employability/ Entrepreneurship/Skill Development

Sr. No.	Course Code	Name of the Course
1.	CMT-101	Analytical Chemistry I
2.	CMT-103	Organic Chemistry I
3.	CMT-105	Polymer Chemistry
4.	CMP-106	Inorganic Chemistry Practical
5.	CMP-107	Organic Chemistry Practical
6.	CMP-108	Physical Chemistry Practical
7.	CMP-109	Analytical Chemistry Practical
8.	CMT-201	Analytical Chemistry II
9.	CMT-203	Organic Chemistry II
10.	CMP-206	Inorganic Chemistry Practical
11.	CMP-207	Organic Chemistry Practical
12.	CMP-208	Physical Chemistry Practical
13.	CMP-209	Analytical Chemistry Practical
14.	CMT-301	Molecular Spectroscopy (Core Paper)
15.	CMT-302	Bio-Molecules and Bio-Catalysts (Core Paper)
16.	CMT-401	Computer Applications in Chemistry (Core Paper)
17.	CMP-409	Project
18.	CMT-305	Forensic Analysis
19.	CMT-405	Environmental Chemistry
20.	CMT-307	Medicinal Chemistry (Core Paper)
21.	CMT-408	Materials Chemistry
22.	CMT -304A	Microanalytical Techniques
23.	CMT -304(O)	Chemistry of Natural Products
24.	CMP -309 (A)	Analytical Chemistry Practical
25.	CMP -309 (I)	Inorganic Chemistry Practical
26.	CMP -309 (O)	Organic Chemistry Practical

27.	CMP -309 (P):	Physical Chemistry Practical
28.	CMT -402 (A)	Separation Techniques
29.	CMT -402 (O)	Application of Spectroscopy to Structural Analysis
30.	CMT -403 (O)	Reagents and Organic Synthesis
31.	CMP-409	Project

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Scheme and Syllabus

Department of Chemistry
School of Physical Sciences
Guru Ghasidas Vishwavidyalya
Bilaspur-495 009

Course structure for M. Sc. (Chemistry

(To be implemented from Session 2012-13)

Semester -I

1 Credit = 1 hour/week

Course Code	Title	Credits
CMT-101	Analytical Chemistry I	3
CMT-102	Inorganic Chemistry I	3
CMT-103	Organic Chemistry I	3
CMT-104	Physical Chemistry I	3
CMT-105	Polymer Chemistry	3
CMP-106	Inorganic Chemistry Practical	2
CMP-107	Organic Chemistry Practical	2
CMP-108	Physical Chemistry Practical	2
CMP-109	Analytical Chemistry Practical	2
	Total:	21+2
	Semester-II	
CMT-201	Analytical Chemistry II	3
CMT-202	Inorganic Chemistry II	3
CMT-203	Organic Chemistry II	3
CMT-204	Physical Chemistry II	3
CMT-205	Chemical Binding	3
CMP-206	Inorganic Chemistry Practical	2
CMP-207	Organic Chemistry Practical	2
CMP-208	Physical Chemistry Practical	2
CMP-209	Analytical Chemistry Practical	2
	Total :	21+2
	Semester-III	
CMT-301	Molecular Spectroscopy (Core Paper)	3
CMT-302	Bio-Molecules and Bio-Catalysts (Core Paper)	3
CMT-303	Specialization Paper-I (A/I/O/P)*	3
CMT-304	Specialization Paper-II (A/I/O/P)*	3
CMT-305-308	Elective Paper I (Any one out of the four papers)+	3
CMP-309	Practical (A/I/O/P)*	6
	Total :	21
	Semester-IV	
CMT-401	Computer Applications in Chemistry (Core Paper)	3
CMT-402	Specialization Paper-I (A/I/O/P)*	3
CMT-403	Specialization Paper-II (A/I/O/P)*	3
CMT-404	Specialization Paper-III (A/I/O/P)*	3
CMT-405-408	Elective Paper II	3
CMP-409	Project	6

I- Inorganic Chemistry O-Organic Chemistry P-Physical Chemistry +4

Elective Papers

+Elective – I		++Elective - II	
CMT-305	Forensic Analysis	CMT-405	Environmental Chemistry
CMT-306	Chemical Applications of Group Theory	CMT-406	Photo Inorganic Chemistry
CMT-307	Medicinal Chemistry (Core Paper)	CMT-407	Bioorganic Chemistry
CMT-308	Physical Methods in Chemistry	CMT-408	Materials Chemistry

* Details of specialization courses are given on the next page

* Details of Specialization Papers

Semester – III

Specialization Papers - I & II

		Credit
Analytical Chemistry		
CMT-303 (A):	Principles of Analytical Chemistry	3
CMT -304 (A):	Microanalytical Techniques	3
Inorganic Chemistry		
CMT -303 (I):	Organometallic Chemistry of Transition Metals	3
CMT -304 (I):	Bio-inorganic Chemistry	3
Organic Chemistry		
CMT -303 (O):	Stereochemistry, Reactions and Rearrangements	3
CMT -304 (O):	Chemistry of Natural Products	3
Physical Chemistry		
CMT -303 (P):	Electrochemistry	3
CMT -304 (P):	Quantum Chemistry	3
CMT 305 Practical		
CMP -309 (A):	Analytical Chemistry Practical	6
CMP -309 (I):	Inorganic Chemistry Practical	6
CMP -309 (O):	Organic Chemistry Practical	6
CMP -309 (P):	Physical Chemistry Practical	6

Semester – IV

Specialization Papers – I, II, III

Analytical Chemistry		
CMT -402 (A):	Separation Techniques	3
CMT -403 (A):	Electroanalytical Methods	3
CMT -404 (A):	Spectrochemical Analysis	3
Inorganic Chemistry		
CMT -402 (I):	Structural Methods in Inorganic Chemistry	3
CMT -403 (I):	Inorganic Rings, Chains, and Clusters	3
CMT -404 (I):	Special Topics in Inorganic Chemistry	3
Organic Chemistry		
CMT -402 (O):	Application of Spectroscopy to Structural Analysis	3
CMT -403 (O):	Reagents and Organic Synthesis	3

CMT -404 (O):	Heterocycles and Vitamins	3
Physical Chemistry		
CMT -402 (P):	Statistical Mechanics	3
CMT -403 (P):	Solid State Chemistry	3
CMT -404 (P):	Chemical Kinetics	3
CMP-409: Project		
CMP -409 (A):	Analytical Chemistry	6
CMP -409 (I):	Inorganic Chemistry	6
CMP -409 (O):	Organic Chemistry	6
CMP -409 (P):	Physical Chemistry	6

Semester- I

CMT-101: Analytical Chemistry-I

Credits: 3

Teaching and learning: To study introduction of analytical chemistry, useful statistical test, Acid-base equilibria treatment in aqueous medium, introduction to chromatographic separation.

1. ***Introduction:*** Scope & objectives, Analytical chemistry and chemical analysis, Classification of analytical methods, Method selection, Sample processing, Steps in a quantitative analysis, Quantitative range (bispartite classification), Data organisation, Analytical validations, Limit of detection and limit of quantitation, The tools of analytical chemistry and good lab practices.

2. ***Analytical chemometrics:*** Useful statistical test: test of significance, the F test, the student 't' test, the chi-test, the correlation coefficient, confidence limit of the mean, comparison of two standard values, comparison of standard deviation with average deviation, comparison of mean with true values, significant figures, regression analysis (least square method for linear and non-linear plots), statistics of sampling and detection limit evaluation. Chemometrics for optimization, modeling and parameter estimation, factor analysis, resolution and pattern recognition.

3. ***Treatment of Equilibria:*** Solvents and solutions, leveling of aqueous and non aqueous solvent effects, general treatment of equilibria in aqueous medium involving monoprotic weak acid and weak base, and salts of weak acids and weak bases. Activity and concentration, Effect of electrolytes on chemical equilibria, Calculation of pH, Constructing titration curves from charge balance and mass balance equations, Acid-base titrations and theory of pH indicators, Complexation equilibria and complexometric titrations, Redox equilibria and redox titration, Theory of redox indicators, precipitation titrations.

4. ***Chromatographic separation:*** Principle of chromatography, classification of chromatography, planar chromatography (paper and thin layer chromatography) and column chromatography (Gas chromatography, High-performance liquid chromatography).

Outcome of teaching -learning:

Students will learn how to do statistical analysis in analytical chemistry for different data analysis, solving problems related to pH and theory of redox indicators, Theoretical approach towards different types of chromatographic separations.

Thermodynamics of mixtures: Thermodynamics of ideal and non-ideal solutions: Liquid-liquid solutions, liquid-solid solutions, multicomponent systems and excess

- Calculate excess thermodynamic properties.
- Solve problems based on Debye-Huckel limiting law. Electrochemistry of solutions, Ion-solvent interactions, ion-ion interactions, ionic migration and diffusion.

Books Recommended

1. *Modern Electrochemistry, Vol. 2 A & B, J.O'M. Bockris and A. K. N. Reddy, Second Edition, Plenum Press, New York (1998).*
2. *Chemical Kinetics, K. J. Laidler,Third Edition (1987), Harper & Row, New York.*
3. *Physical Chemistry, P. W. Atkins, 7th Edition, Oxford University Press, New York (2002)*
4. *Physical Chemistry, P. W. Atkins, 7th Edition, Oxford University Press, New York (2002).*
5. *Physical Chemistry, I.N. Levine, 5th Edition (2002), Tata McGraw Hill Pub. Co. Ltd., New Delhi.*
6. *Kinetics and Mechanism of Chemical Transformations, J. Raja Ram and J.C. Kuriacose, MacMillan Indian Ltd., New Delhi (1993).*

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CMT-105: Polymer Chemistry

Credits: 3

Teaching and learning: To get the knowledge about introduction of polymers, Mechanism ad kinetics of polymerization, polymer structures and properties.

1. Introduction, Classification of Polymers, Intermolecular forces in Polymers.
2. **Mechanism and kinetics of step-growth and chain growth polymerization:** radical, cationic, anionic and condensation polymerization. Copolymerization, Reactivity Ratios, Thermodynamic Aspects of Polymerization. Mechanism of Living Radical Polymerizations: Nitroxide mediated polymerization (NMP), Metal-catalyzed Living Radical Polymerization, Coordination polymerization, Ring opening polymerization,
3. **Polymer solutions:** Thermodynamics of polymer dissolution, The Flory-Huggins Theory of Polymer solutions, Nature of polymer macromolecules in solution, Size and shape of macromolecules in solution.
4. **Polymer structure and Physical properties:** Microstructure of polymer chains, crystallinity in polymers, Glass transition temperature, rheological properties. Degradation of polymers. Polymer reactions. Polymer Processing
5. **Experimental methods:** polymer fractionation, molecular weight determination: Molecular mass – number and mass average molecular mass, determination of molecular mass by Osmometry, viscosity, light scattering and size exclusion chromatography.

Outcome of teaching -learning:

- Students should be able to apply the different molecular weights and methods of determination to synthesized new polymers
- To apply the Mechanisms and Methods of Polymerization - Step (condensation) polymerization - Description - Molecular weight distribution. Chain polymerization, controlled radical polymerizations (ATRP, RAFT,). Living Polymerizations.
- Students should be able to understand the structure and physical properties of polymers

Books Recommended

1. *F. W. Billmayer, Jr., Text Book of Polymer Science, 3rd Edition (1984), Willey-Interscience, New York.*
2. *G. Odian, P. W. Atkins, Physical Chemistry, 6th Edition, Oxford University Press, New York.*
3. *G. Odian, Principles of Polymerization, 3rd edition (1991) John Wiley, Singapore*
4. *P.Bahadur and N.V. Sastry, Principle of Polymer Sciences , Narosa Publishing House, New Delhi (2002)*
5. *V.R. Gowarikar, N.V. Vishwanathan, J. Shreedhar , Polymer Sciences, Wiley Eastern, New Delhi (1986)*

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Practical

CMP-106: Inorganic Chemistry Practical

Credits: 2

Teaching and learning: The learners should be able to validate the conceptual understanding acquired from the theory classes

1. Quantitative separation and determination of the following pairs of metal ions using gravimetric and volumetric methods:

   (i) Ag^{+} (gravimetrically) and Cu^{2+}(Volumetrically)
   (ii) Cu^{2+} (gravimetrically) and Zn^{2+}(Volumetrically)
   (iii) Fe^{3+} (gravimetrically) and Ca^{2+}(Volumetrically)
   (iv) Mg^{2+} (gravimetrically) and Ca^{2+}(Volumetrically)

2. Separation of a mixture of cations/anions by paper chromatographic technique using aqueous/non-aqueous media.

   (i) Pb^{2+} and Ag^{+} (aqueous and non-aqueous media)
   (ii) Co^{2+} and Cu^{2+} (non-aqueous medium)
   (iii) Cl^{-} and I^{-} (aqueous-acetone medium)
   (iv) Br^{-} and I^{-} (aqueous-acetone medium)

Outcome of teaching -learning:

On successful completion of these semesters, students will be able to know:

- The principles and applications of qualitative and quantitative analysis.
- Learning paper chromatographic techniques for the identification and separations of inorganic cations/anions.
- Techniques and analysis of minerals and ores
- Collection, analysis and representation of data in a scientific manner

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CMP-107: Organic Chemistry Practical

Credits: 2

Teaching and learning: The learners should be able to validate the conceptual understanding acquired from the theory classes.

Separation of binary mixtures (Solid-Solid) of organic compounds and identification of individual components (physical characterization, elemental analysis, functional group (s) detection, derivative preparation and melting point determination

Outcome of teaching -learning:

On Completion of this module, the learner will be able to:

- Independently identify the presence of different components/molecules in the unknown organic mixture
- Detection of elements, functional groups,
- Prepare derivatives of organic molecules

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CMP-108: Physical Chemistry Practical

Credits: 2

Teaching and learning: The learners should be able to validate the conceptual understanding acquired from the theory classes

1. Saponification of ethyl acetate with sodium hydroxide by chemical method.
2. Comparison of acid strengths through acid catalyzed methyl acetate hydrolysis.
3. Energy of activation of acid catalyzed hydrolysis of methyl acetate.
4. Distribution coefficient of I_2 between two immiscible solvents.
5. Conductometric titration of a weak acid with strong base.
6. Conductometric titration of a mixture of weak and strong acids.
7. Potentiometric titration of a strong acid with strong base using quinhydrone electrode.
8. Conductometric titration of KCl with $AgNO_3$.
9. Molecular weight of a non-electrolyte by cryoscopy method.
10. Determination of Molecular weight of a non volatile substance (non electrolyte) by Landberger method.

Outcome of teaching -learning:

At the end of the course, the learners should be able to: Explain the principle behind the experiments performed in the laboratory Plan and Perform experiments and Interpret experimental results

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CMP-109 (A): Analytical Chemistry Practical

Credits: 2

Teaching and learning: The learners should be able to validate the conceptual understanding acquired from the theory classes

1. Determination of accuracy, precision, standard deviation, coefficient of variation, and least square fitting of certain set of experimental data in an analysis
2. Composition of two sets of results in terms of significance (Precision and accuracy) by (i) student's t-test, (ii) F-test
3. Quantitative determination of iron in soil samples by Redox titration method
4. Determination of hardness by EDTA titrations method using Eriochrome Black T
5. Determination of chloride by Argentometric method
6. Determination of composition of the metal complexes by Jobs continuous variation and mole ratio method
7. Spectrophotometric determination of iron using thiocyanate method
8. Determination of buffer capacity by pH metry.

Outcome of teaching -learning:

On successful completion of these semesters, students will be able to know:

- The principles and applications of instrumental methods of analysis, including chemical separation methods etc.
- formulating and solving problems in the laboratory
- how to communicate scientific information clearly and accurately, both in oral and in written forms
- the composition of written laboratory reports that summarize experimental procedures and the accurately present and interpret data
- statistical methods of data analysis including error distributions, hypothesis testing, confidence intervals, the method of maximum likelihood or least-squares analysis.

Note: Experiments may be added/deleted subject to availability of time and facilities.

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Semester-II

CMT-201: Analytical Chemistry-II

Credits: 3

Teaching and learning: To study the principles and instrumentation of various techniques such as polarography, AAS, AFS, AES, spectrophotometry, thermal analysis (TGA, DTA & DSC), Automation in lab.

1. ***Polarography:*** Origin of polargraphy, Current-voltage relationship, Theory of polarographic waves (DC and sampled DC (tast) polarograms), Instrumentation, interpretation of polarographic curve, Limiting current, residual and charging current, diffusion current, migration current. Supporting electrolytes. Effect of supporting electrolyte on the limiting current, Half wave potential and its significance, Qualitative and quantitative applications.

2. ***Spectroscopic Techniques:*** Theory, Instrumentation and applications of X-rays (emission, absorption, diffraction and fluorescence methods), Atomic absorption Spectroscopy, Atomic fluorescence spectrometry, Atomic emission spectrometry.

3. ***Spectrophotometry***: UV-visible molecular absorption spectrometry, Principle and applications, determination of stoichiometry of complexes (Job's method of continuous variation, mole ratio and slope ratio analysis). Molecular luminescence spectrometry (fluorescence, phosphorescence, chemiluminescence).

4. ***Thermal Analysis:*** Theory, methodology and applications of thermogravimetric analysis (TGA), Differential Thermal Analysis (DTA), and Differential scanning calorimetry (DSC). Principles, techniques and applications of thermometric titration methods

5. ***Automation in the Laboratory***: Principles of automation, Process control through automated instruments, Autoanalyzers (single channel and multi-channel), Basic sequences of multi-fold operational analyzers in segmented and non-segmented flows.

Outcome of teaching -learning:

Having successfully completed this module, you will be able to:

- understand the underlying theoretical basis of analytical techniques including titration and gravimetric analysis, spectroscopic methods including UV-visible, Fluorescence, and atomic absorption, chromatography, and electroanalysis;
- be able to select the appropriate analytical methods to evaluate a sample;
- critically evaluate data from a variety of analytical chemistry techniques and apply knowledge of the statistical analysis of data;
- have developed the skills required to work as a member of a group;
- be aware of current developments in the field of analytical chemistry.

Books Recommended

1. *Willard, Merrit, Dean, Settle, Instrumental Methods of Analysis, 7th Edition, CBS Publishers & Distributors PVT Ltd.*
2. *D.A. Skoog, Principles of Instrumental Analysis, 5th Edition (1998), Saunders College Publishing, Philadelphia, London.*
3. *R.L. Pecsok, L. D. Shields, T. Cairns and L.C. Mc William, Modern Methods of Chemical Analysis, 2nd Edition (1976), John Wiley, New York.*
4. *J.H. Kennedy, Analytical Chemistry: Principles, 2nd Edition (1990), Saunders Holt, London.*
5. *G. D. Christian, Analytical Chemistry, 5th Edition (1994), John Wiley & Sons, New York.*

CMT-202: Inorganic Chemistry-II

Credits: 3

Teaching and learning: To understand the nature of substitution reactions in metal complexes of different geometry. Knowing about one of the important reactions i.e. electron transfer reactions and related theory.

1. **Kinetics and Mechanism of Substitution Reactions:** Nature of substitution reactions; prediction of reactivity of octahedral, tetrahedral and square-planar complexes in terms of VBT and CFT; rates of reactions; acid hydrolysis, base hydrolysis and anation reactions.

2. **Electron Transfer Reactions:** Mechanism and rate laws; various types of electron transfer reactions, Marcus-Husch theory, correlation between thermal and optical electron transfer reactions.

3. **Transition Metal π-acid Complexes**
Bonding, synthesis and reactivity of transition metal complexes with CO, NO, metal carbonyl hydrides and metal carbonyl clusters: Wade's rule and the capping rule.

4. **Supramolecular chemistry**: Definition, supramolecular host-guest compounds, macrocyclic effect, nature of suparmolecular interactions, molecular machine, biomodelling.

5. **Optical Rotatory Dispersion and Circular Dichroism :** Basic Principles of ORD and CD techniques. ORD and Cotton effect, Faraday and Kerr effects; Applications in determining absolute configuration of metal complexes.

Outcome of teaching -learning:

After successfully completion this module, the students will be able to:

- Understand the nature of substitution reactions in metal complexes.
- Use of electron transfer reaction to fabricate solar cell.
- Develops better understanding for electron transfer reaction in biological system.
- Have developed the skills required to work as a member of a group.
- Keeping update of current developments in the field of inorganic chemistry.

After successful completion of the course, students will learn the advanced organic chemistry concepts that will be applied in solving their future chemistry problems. They will learn about Arenium ion mechanism, orientation and reactivity. participation by π and σ bonds, Anchimeric assistance. Classical versus non-classical carbonium ions. Woodward-Hoffmann rules; cycloaddition [2+2] and [4+2], and electrocylic reactions. Prototropic and Sigmatropic rearrangements, Ene reactions and Cheletropic reactions; 1,3-Dipolar cycloaddition. Photochemical energy, Jablonski diagram, photosensitisation and quenching, Isomerization, Di-π-methane rearrangement and cycloadditions; Norrish type-I and Norrish type-II cleavage; Paterno-Buchi reaction, photodimerisation of α,β-unsaturated ketones, rearrangement of enones and dienones, Photo-Fries rearrangement.

Books recommended

1. *M.B. Smith & Jerry March, March's Advanced Organic Chemistry, 5th Edition (2001), John Wiley & Sons, New York.*
2. *Peter Sykes, A Guide Book to Mechanism in Organic Chemistry, 6th Edition (1997), Orient Longman Ltd., New Delhi.*
3. *S.M. Mukherjee and S.P. Singh, Reaction Mechanism in Organic Chemistry, Ist Edition (1990), Macmillan India Ltd., New Delhi.*
4. *T.H. Lowry and K.S. Richardson, Mechanism and Theory in Organic Chemistry, 3rd Edition (1998), Addison – Wesley Longman Inc. (IS Edition).*
5. *R.T. Morrison and R.N.Boyd, Organic Chemistry, 6th Edition (2003), Prentice- Hall of India, New Delhi.*
6. *P. S. Kalsi, Organic Reactions and Their Mechanisms, Ist Edition (1996), New Age International Pub., New Delhi.*
7. *S. M. Mukherjee and S. P. Singh, Pericyclic Reactions, MacMillan India, New Delhi.*
8. *I. Fleming, Pericyclic Reactions (1999), Oxford University Press, Oxford.*
9. *I. Fleming, Frontier Orbitals and Organic Chemical Reactions (1976), Wiley, New York.*
10. *T. L. Gilchrist and R. C. Storr, Organic Reactions and Orbital Symmetry, 2nd Edn., Cambridge University Press, 1979.*
11. *R.B. Woodward and R. Hoffman, The Conservation of Orbital Symmetry, Verlag Chemie GmbH, 1970.*
12. *T.H. Lowry and K.C. Richardson, Mechanism and Theory in Organic Chemistry, 3rd Edn., Harper and Row, 1998.*
13. *J. Singh and J. Singh, Photochemistry and Pericyclic Reactions, 2nd Edn., New Age International (P) Ltd., 2005*
14. *John D. Coyle, Introduction to Organic Photochemistry, John Wiley and Sons, New York (1986).*
15. *C. H. Depuy and O. L. Chapman, Molecular Reactions and Photochemistry, 2nd Edition (1988), Prentice-Hall of India (P) Ltd., New Delhi.*
16. *F. A. Carey and R. J. Sundberg, Photochemistry in Advanced Organic Chemistry, Chapter 13, Part A, 3rd Edition (1990), Plenum Press, New York.*
17. *N. J. Turro, Modern Molecular Photochemistry, University Science Books, Sausalito (1991).*

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CMT-204: Physical Chemistry-II

Credits: 3

Teaching and learning: To learn the basic concept of Corrosion and micelles and their uses, radio chemistry and transport phenomenon like viscosity, diffusion etc in gaseous state, learn the micelles.

1. **Corrosion:** Scope and economics of corrosion, causes and types of corrosion, electrochemical theories of corrosion, kinetics of corrosion (corrosion current and corrosion potential). Corrosion measurements (weight loss, OCP measurement, and polarization methods), units of corrosion rate, passivity and its breakdown. Corrosion prevention (electrochemical, inhibitor, and coating methods).
2. **Transport Phenomena:** *General transport equation*: Thermal condutivity, Viscosity and

Diffusion. *Intermolecular Forces*: Long range forces. Lennard Jones potential. **Physical transformation of Pure substances:** stability of Phases, Phase boundaries, three typical phase diagram, thermodynamic criteria of equilibrium, the dependence of the stability on the conditions, location of phase boundaries, the Ehrenfest classification of phase transition.

3. **Chemical thermodynamics**: Laws, state and path functions and their applications; thermodynamic description of various types of processes; Maxwell's relations; spontaneity and equilibria; temperature and pressure dependence of thermodynamic quantities; Le Chatelier principle; elementary description of phase transitions; phase equilibria and phase rule; thermodynamics of ideal and non-ideal gases, and solutions.

4. **Micelles** Surface-active agents and their classification, Hydrophile-Lipophile Balance: HLB parameter, Shape and Structure of micelles, micro-emulsions, reverse micelles, micellization, Critical micceller concentration (cmc), phase separation and mass action models, factors affecting cmc of surfactants, thermodynamics of micellization, micelle temperature range: MTR or Krafft Point.

5. **Radiochemistry:** Radiation detection & measurements--Proportional, Geiger-Muller and Scintillation counters, semiconductor detectors. Radiochemical principles in the use of tracers. Applications of radioisotopes as tracers: activation analysis, isotope dilution technique, age determination, medical applications, and some agricultural applications. *Radiation Chemistry*: Elements of radiation chemistry, units for measuring radiation absorbed.

Outcome of teaching -learning:

- Different types of corrosion; influence of environment; corrosion rate measurements; mixed potential theory and prevention of corrosion.
- Students should be able to understand the details of surfactants
- Students should be able to understand the formation of micelles its thermodynamic outcome, hydrophobic interaction
- Students should be able to use the different detectors to perform the radiochemical reaction
- Students should be able to understand the thermodynamic in daily life

Books Recommended

1. *Modern Electrochemistry, Vol. 2 A & B, J.O'M. Bockris and A. K. N. Reddy, Second Edition, Plenum Press, New York (1998).*
2. *Electrochemical Methods: Fundamentals and Applications; A.J. Bard and L.R. Faulkner, 2nd edition (2001), John Wiley & Sons, New York.*
3. *Physical Chemistry, P. W. Atkins, 7th Edition, Oxford University Press, New York (2002).*
4. *Physical Chemistry, N. Levine, 5th Edition (2002), Tata McGraw Hill Pub. Co. Ltd., New Delhi.*
5. *"Physical Chemistry", K. J. Laidler and J. M. Meiser, 3rd Edition (International Ed.) Houghton Mifflin Co., New York.*
6. *"Physical Chemistry", R. S. Berry, S. A. Rice and J. Ross, 2nd Edition, Oxford University Press, Oxford (2000).*
7. *Y. Moroi, Micelles: Theoretical and Applied Aspects, Plenum Press, New York (1992).*
8. *F.W. Billmayer, Jr., Text Book of Polymer Science, 3rd Edition (1984), Wiley-Interscience, New York.*
9. *B. G. Harvey, Introduction to Nuclear Physics and Chemistry, Prentice Hall, Inc. (1969).*
10. *H.J. Arnikar, Essentials of Nuclear Chemistry, 4th Edition (1995), Wiley-Eastern Ltd., New Delhi.*
11. *G. Fridlander, J.W. Kennedy, E. S. Macias, and J. M. Miller, Nuclear & Radiochemistry, 3rd*

Practical

CMP-206: Inorganic Chemistry Practical

Credits: 2

Teaching and learning: The learners should be able to validate the conceptual understanding acquired from the theory classes

1 Preparation of coordination complexes and their characterization by magnetic susceptibility measurements and IR, UV / Vis, ^{1}H NMR spectroscopic techniques.

Outcome of teaching -learning:

On successful completion of this sem, students will be able to know:

- Practical idea about complex compound and its properties.
- Knowing and able to interpret the spectral properties of metal complexes.
- Naming coordination compounds and to be able to draw the structure based on it's name.
- Collection, analysis and representation of data in a scientific manner.

CMP-207 Organic Chemistry Practical

Credits: 2

Teaching and learning: The learners should be able to validate the conceptual understanding acquired from the theory classes

1. Synthesis of organic compounds involving important chemical reactions such as nitration, bromination, diazotization & coupling reactions, molecular rearrangements etc.
2. Isolation of some natural products (Caesin from milk, lycopene from tomatoes, Nicotine from tobacco leaves etc.) and characterization using FT-IR, UV-Vis spectroscopy.

Outcome of teaching -learning:

On Completion of this module, the learner will be able to:

- Independently synthesize important organic molecules
- Purify synthesized molecules
- Calculate the percentage of yield of the products
- Able to identify the outcome of products by spectroscopic techniques

CMP-208 Physical Chemistry Practical

Credits: 2

Teaching and learning: The learners should be able to validate the conceptual understanding acquired from the theory classes.

1. Rate constant of acid catalyzed hydrolysis of sucrose by polarimetric method.
2. Rate constant of acid catalyzed hydrolysis of sucrose by chemical method.
3. Rate constant of $FeCl_3$-catalyzed H_2O_2 decomposition by gasometric method.
4. Degree of hydrolysis of urea hydrochloride by kinetics method.
5. Equilibrium constant of $KI + I_2 = KI_3$ by distribution method.
6. Phase diagram of a binary organic system (Naphthalene and Diphenyl).
7. Determination of solubility and solubility product of sparingly soluble salt

conductometrically.

8. Potentiometric titration of a redox system (ferrous ammonium sulfate with $K_2Cr_2O_7$).
9. Adsorption of acetic acid on charcoal to verify Freundlich adsorption isotherm.
10. Determination of the velocity constant of hydrolysis of an ester/ionic reaction in miceller media.

Outcome of teaching -learning:

At the end of the course, the learners should be able to explain the principle behind the experiments performed in the laboratory plan and perform experiments and Interpret experimental results.

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CMP-209 (A): Analytical Chemistry Practical

Credits: 2

Teaching and learning: The learners should be able to validate the conceptual understanding acquired from the theory classes

1. Determination of biological oxygen demand (BOD) and dissolved oxygen (DO) in water samples
2. Determination of chemical oxygen demand (COD) in waste water samples
3. Determination of total phosphorous and total dissolved solid in drinking water
4. Gas chromatography: Quantitative determination of organic compounds
5. Thin layer chromatography: Separation of amino acids
6. Iodometric titration: Determination unsaturation (iodine number)
7. Potentiometric titration: Determination of concentration of halide ion(s) in given solution
8. Determination of trace metal impurities present in water sample by voltammetric method

Outcome of teaching -learning:

On successful completion of this semester, students will be able to know:

- The principles and applications of chromatographic separation methods etc.
- formulating and solving problems based on objectives given in the laboratory
- statistical methods of data analysis including error distributions, hypothesis testing, confidence intervals, the method of maximum likelihood or least-squares analysis

Note: Experiments may be added/deleted subject to availability of time and facilities.

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Semester-III

CMT-301: Molecular Spectroscopy

(Core Paper)

Credits: 3

Teaching and learning: To study absorption and emission of radiation. Selection rules. Line

shapes and widths. Fourier transform spectroscopy, Basic concepts of rotational and vibrational spectroscopy, Instrumentation, basic principle, techniques and applications of NMR, Concept of electronic and photoelectron spectroscopy.

1. **Time-dependent states and spectroscopy**: absorption and emission of radiation. Selection rules. Line shapes and widths. Fourier transform spectroscopy

2. **Rotation and Vibration of Diatomic Molecules:** Vibration-rotational spectra of diatomics; P.Q,R branches, normal modes of vibration, overtones, hot bands Raman spectroscopy: Origin; rotational and vibrational Raman spectra of diatomics, Anharmonicity, Selection Vibration of polyatomic molecules–normal coordinates. Polarization of Raman lines. Fingerprint region and applications

3. **Electronic spectroscopy:** Electronic spectra of diatomic molecules, Franck-Condon principle, Vibronic transitions, $\pi \rightarrow \pi^*$, $n \rightarrow \pi^*$ transition. Dissociation and pre-dissociation. Rotational fine structure

4. **Nuclear Magnetic Resonance:** Review of angular momentum. Basic principles and relaxation times. Magnetic resonance spectrum of hydrogen. First-order hyperfine energies. NMR in liquids: Chemical shifts and spin-spin couplings First order Spectra: A_3X, AX and AMX systems. Solid state NMR spectroscopy, Introduction of 2D NMR spectroscopy, Basic principle and Applications of COSY, NOE and HMBC.

5. **Photoelectron Spectroscopy (PES):** Photo excitation and photo ionization, core level photo ionization (XPS, ESCA.) and valence level (UPS) experiments, detection of atoms in molecules, chemical shift.

Outcome of teaching -learning:

- Students will learn absorption and emission of radiation. Selection rules. Line shapes and widths. Fourier transform spectroscopy
- Students will learn Basic concepts of rotational and vibrational spectroscopy
- Instrumentation, basic principle, techniques and applications of NMR
- Concept of electronic and photoelectron spectroscopy

Book Recommended

1. *J. M. Hollas, Modern Spectroscopy, 4th edition (2004) John Wiley & Sons, Ltd., Chichester.*
2. *C. N. Banwell and E.M. Mc Cash, Fundamentals of Molecular Spectroscopy, 4th edition (1994), Tata McGraw Hill, New Delhi.*
3. *A Carrington and A. D. Mc Lachlan, Introduction to Magnetic Resonance, Chapman and Hall, London (1979).*
4. *R. K. Harris, Nuclear Magnetic Resonance Spectroscopy, Addison Wesley, Longman Ltd, London (1986).*

CMT-302: BIOLOGICAL CHEMISTRY

Credits: 3

Teaching and learning: Students will get the knowledge of life-molecules, structures and function, metabolism and energetics, enzymes and metalloenzymes, molecular recognition.

1. **Molecules of life**: Amino acids and proteins, Carbohydrates-polysaccharides, lipids, cell-membranes and nucleic acids

2. **Structure and function**: Protein structure, Ramachandran - plot, protein folding: DNA/RNA structures, various forms (a, b, c, z) of DNA, t-RNA structure, transcription and translation,

gene expression and DNA binding protein-zinc-finger protein.

3. **Metabolism and Energetics**: Glycolysis , citric acid cycle , oxidative phosphorylation and transport through membranes

4. **Enzymes:** Introduction, classification, formation and function of enzymes, co-enzymes, cofactors (elementary idea); Enzyme kinetics, TON and TOF, Enzyme inhibitors.

5. **Metalloenzymes**: Hydrolytic and redox enzymes: Carbonic anhydrase and superoxide dismutase

6. **Oxygen uptake proteins**: Hemerythrin and hemocyanin

7. **Molecular recognition**: Molecular organization, Chiral recognition and role of sugar in biological recognition.

Outcome of teaching -learning:
Students will explain and describe the synthesis of amino acids, proteins including their structures, lipids, nuclic acids, carbohydrates, metallo proteins, metallo enzymes and their role in metabolic pathways. They also learn in details about types of enzyme, enzyme kinetic reaction, inhibition of enzyme kinetic reactions, inhibitors, glycolysis, citric acid cycle, phophorylations and molecular recognitions.

Books Recommended

1. *L. Stryer, Biochemistry, 5th Edition, (2002) Freeman &Co. New York*
2. *D.L. Nelson and M.M. Cox, Lehninger Principles of Biochemistry 3rd Edition ((2002) McMillan North Publication*
3. *D. Voet, J. G. Voet, Biochemistry 3rd Edition (2004), Wiley International Publication.*
4. *I. Bertini, H. B. Gray, S. J. Lippard, J.S. Valentine, 1st South Asian Edn., (1998) Viva Books Pvt. Limited, New Delhi*
5. *M. B. Smith, Organic Synthesis, (1998) Mc Graw Hill Inc, New York*

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Specialization Papers I & II
Analytical Chemistry Specialization

CMT-303 (A): Principles of Analytical Chemistry

Credits: 3

Teaching and learning: Study of acid-based equilibria treatment in aqueous medium, pH calculation, introduction to buffer solution and applications, pH calculations, photometric titrations, Construction and applications of different types of sensors.

1. **Acid-Base Equilibria:** General concept of acid-base equilibria in water and in non-aqueous solvent, Definition of pH and pH scale (Sorenson and operational definitions), and its significance, Hammett acidity function, pH calculation for aqueous solutions of very weak acid and very weak base, salts of weak acid and weak bases, mixture of weak acid and its salts, mixture of weak base and its salts.

2. **Buffer Solutions:** Theory of buffer solution, dilution and salts effects on the pH of a buffer, Buffer index, Criteria and expression of maximum buffer capacity, Application of

pH buffers, Preparation of buffer solutions of known ionic strength (Typical examples). Practical limitations in use of buffers, Metal ion buffers and their applications, Biological buffers and their applications.

3. **Photometric Titrations:** Basic principles, comparison with other titrimetric procedures, types of photometric titration curves, Instrumentation (Titration cell, Detectors, choice of analytical wavelength). Quantitative applications, Typical examples of one component and multicomponent analyses.

4. **Chemical Sensors:** Principles, types of chemical sensors based on the modes of transductions, Types of chemical sensor based on the chemically sensitive materials (solid electrolyte, gas, semiconductor), Humidity sensors, Biosensors, Electrochemical sensors (Potentiometric sensors, Ion-selective electrodes, Membrane electrodes, Amperometric sensors, Clark and Enzyme electrodes).

Outcome of teaching -learning:

Student will learn theoretical approach to acid-base equalibria treatments in aqueous medium and calculation of pH, buffer system, construction and applications of different types of electrochemical, optical, mass sensor etc.

Books Recommended

1. D.A. Skoog and D.M. West, *Fundamental of Analytical Chemistry*, International Edition, 7thEdition (1996), Saunders College Publishing, Philadelphia, Holt, London.
2. R.L. Pecsok, L.D. Shields, T. Cairns and L.C. McWilliam, *Modern Methods of Chemical Analysis*, 2nd (1976), John Wiley & Sons, New York.
3. D.A. Skoog, *Principles of Instrumental Analysis*, 5th Edition (1998), Saunders College of Publishing, Philadelphia, London.
H.A. Strobel, *Chemical Instrumentation: A Schematic Approach*, 2nd Edition (1973), Addison Wesley, Reading, Mass

References

1. H.A. Laittnen and W.E. Harris, *Chemical Analysis*, 2nd International Student Edition (1960), McGraw Hill, New York.
2. R.G. Bates, *Electrometric pH Determinations: Theory and Practice*, 3rd Edition (1973), John Wiley & Sons, New York.
3. G.D. Moody and J.D.R. Thomas, *Ion-selective Electrodes*, London.
4. G.W. Ewing, *Instrumental Methods of Chemical Analysis*, 5th Edition (1978), McGraw Hill Book Co., New York.

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CMT-304(A): Chemical Analysis

Credits:3

Teaching and learning: The primary objective of this course is to acquire basic concepts, principles, and techniques of modern analytical chemistry that would empower students with an analytical mind set and the abilities to solve diverse analytical problems in an efficient and quantitative way that conveys the importance of accuracy and precision of the analytical results.

1. **Sampling, Standardization & Calibration:** Analytical samples and methods, sampling and sample handling of minerals, ores, metals, liquid, gaseous, solids and biological samples, obtaining a representative sample, sampling uncertainties, the gross sample, preparing a laboratory sample, standardization and calibration, comparison with standards, external standard calibration, minimizing errors in analytical procedures.

2. **Molecular recognition and applications:** Definition and principle of recognition process, host guest interaction, receptor in separation of cation and anions, crown ethers, cryptands, calixarenes.

3. **Biochemical analysis:** Estimation of carbohydrates, amino acids and ascorbic acid in biological systems, purification of proteins (spectrophotometric and ELISA), estimation of protein in egg albumin, estimation of free fatty acid, Iodine value and saponification value of fats/oils, estimation of blood cholesterol, DNA and RNA.

4. **Soil and water analysis:** Determination of nitrogen, phosphorus (spectrophotometric), potassium, calcium, sodium (flame photometric) in soil samples; determination of metals, iron, copper, nickel and zinc (spectrophotometric) arsenic, lead, mercury, chromium, selenium (AAS) in soil and water samples.

5. **Organic group analysis:** Determination of hydroxyl, carbonyl, amides and ester groups, Determination of molecular weight and percentage purity of carboxylic acid, Estimation of sugars, Estimation of unsaturation.

Outcome of teaching -learning:

The student learns the skill to prepare standard solution, samples and analysis of the samples through using accurate methods. The course makes the student to learn how to prepare solutions quantitatively and analysis the analyte with high accuracy.
Therefore, students will be able:

- To develop an understanding of the range and uses of analytical methods in chemistry.
- To establish an appreciation of the role of chemistry in quantitative analysis
- To develop an understanding of the broad role of the chemist in measurement and problem solving for analytical tasks.
- To provide an understanding of chemical methods employed for elemental and compound analysis.
- To provide experience in some scientific methods employed in analytical chemistry.
- To develop some understanding of the professional and safety responsibilities residing in working on chemical analysis.

Books Recommended

1. *P.L. Kirk, Quantitative Ultramicroanalysis, John Wiley.*
2. *C.L. Wilson and D.L. Wilson, Comprehensive Analytical Chemistry", Vol. I (A) and I(B), Elsevier.*
3. *G.D. Christian, Analytical Chemistry, John Wiley & Sons, New York (2001).*
4. *S.M. Khopkar, Analytical Chemistry of Macrocyclic and Supramolecular Compounds, Narosa Publishing House, New Delhi (2002).*
5. *Jag Mohan, Organic Analytical Chemistry - Theory and Practice, Narosa Publishing House, New Delhi (2003).*

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Inorganic Chemistry Specialization
CMT-303 (I): Organometallic Chemistry of Transition Metals

Credits: 3

Teaching and learning: A brief study of metal carbonyls, role of transition metal compounds in catalysis, porous materials organic-inorganic hybrid materials.

1. **Metal Carbonyls:** Dioxygen and Dinitrogen, Semibridging carbonyl group; metal nitrosyl carbonyls; tertiary phosphines and arsines as ligands; carbenes and carbynes.
2. **Transition Metal Compounds in Catalysis**: Hydrogenation, hydroformylation and polymerization; Waker process, Monsanto process.
3. **Transition Metal Compounds with M-H bonds**: Metal hydrides (classical and non-classical). Agostic interaction. Application of NMR in studying hydrido complexes.
4. **Porous materials Organic-inorganic hybrid materials**: Zeolites, AlPO, mesoporous materials, Soft chemistry-based processes, functionalization of porous materials, MOF compounds.

Outcome of teaching -learning:

- Student will learn the use of organometallic catalysis in manufacture of different organic compounds by hydrogenation, hydroformylation and polymerization; Waker process, Monsanto process the etc.
- Will be able to know about classical and non-classical metal hydrides, agnostic interactions and proton NMR in studying hydrido complexes.
- Knowing about preparation, properties and applications of porous materials.

Books Recommended

1. F. A. Cotton and G. Wilkinson, *Advanced Inorganic Chemistry*, 6th Edn., (1999), John-Wiley & Sons, New York.
2. James E. Huheey, *Inorganic Chemistry*, 4th Edn., (1993), Addison Wesley Pub. Co., New York.
3. R. H. Crabtree, *The Organometallic Chemistry of the Transition Metals*, 1st Edn.(1988), John-Wiley & Sons, New York.
4. J. P. Collman, L. S. Hegedus, J. R. Norton and Richard G. Finke, *Principles and Applications of Organotransition Metal Chemistry*, 1st Edn.(1987), University Science Books, Mill Valley.
5. Ch. Elschenbroich and A. Salzer, *Organometallics*, VCH.
6. C. N. R. Rao, J. Gopalakrishnan, *New Directions in Solid State Chemistry; Cambridge University Press*: Cambridge (1997).
7. A. K. Cheetham, *Solid State Chemistry:Compounds*; Oxford University Press: Oxford, (1992).
8. J. N. Lalena and D. A. Cleary, *Principles of Inorganic Materials Design*; Wiley: New York, (2010).

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CMT-304 (I): Bio-inorganic Chemistry

Credits: 3

Teaching and learning: A vast knowledge about Iron, copper and molybdenum proteins with reference to their oxygenation and oxidase activity: (i) Anti-oxidative functions: cytochrome P-450, catalases and peroxidases, (ii) Nitrate and nitrite reduction: NO_3 and NO_2 reductase, (iii) Electron transfer: cytochromes; blue copper proteins and iron-sulfur proteins and their Synthetic models, (iv) Nitrogen fixation through metal complexation, nitrogenase, (v) Photosynthesis (PS-I and PS-II). Iron storage and transport proteins: Ferritin, Transferritin and Hemosiderin

1. **Role of alkaline earth metal ions in biological systems :** (i) Catalysis of phosphate transfer by Mg^{2+} ion, (ii) Ubiquitous regulatory role of Ca^{2+} -muscle contraction.
2. **Iron, copper and molybdenum proteins with reference to their oxygenation and oxidase activity:** (i) Anti-oxidative functions: cytochrome P-450, catalases and peroxidases, (ii) Nitrate and nitrite reduction: NO_3 and NO_2 reductase, (iii) Electron transfer: cytochromes; blue copper proteins and iron-sulfur proteins and their Synthetic models, (iv) Nitrogen fixation through metal complexation, nitrogenase, (v) Photosynthesis (PS-I and PS-II).
3. **Metalloenzymes:** Urease, Hydrogenase, and Cyanocobalamine.

4. **Interaction of metal complexes with DNA:** DNA probe and chemotherapeutic agents.
5. **Iron storage and transport proteins:** Ferritin, Transferritin and Hemosiderin

Outcome of teaching -learning:

- Student will learn biological process and application of different enzymes in it.
- Understanding electron transfer reactions in biological process.
- Knowing about biological nitrogen fixation and photosynthetic process and its synthetic models.
- Transport of iron in micro- and macro-organism.

Books recommended

1. *M. N. Hughes, Inorganic Chemistry of Biological Processes, 2nd Ed.(1981), John-Wiley & Sons, New York.*
2. *W. Kaim and B. Schwederski, Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, An Introduction and Guide, Wiley, New York (1995).*
3. *S. J. Lippard and J. M. Berg, Principles of Bioinorganic Chemistry, University Science Books, (1994).*
4. *I. Bertini, H. B. Grey, S. J. Lippard and J. S. Valentine, Bioinorganic Chemistry, Viva Books Pvt. Ltd., New Delhi (1998).*

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ORGANIC CHEMISTRY SPECIALIZATION

CMT-303(O): STEREOCHEMISTRY, REACTIONS & REARRANGEMENTS

Credits: 3

Teaching and learning: A detailed study of stereochemistry and conformations in organic molecules, asymmetric synthesis, various name reactions and rearrangements.

1. **Stereochemistry**: Molecular symmetry and chirality; stereoisomerism: definitions, classifications; configuration and conformation; relative and absolute configuration; determination of relative configuration: Prelog's rule, Cram's rule (Felkin modification), and Sharpless rule; Chiral auxiliaries, Optical Activity in absence of chiral carbon: biphenyls and Allenes and Atropisomerism.

2. **Asymmetric Synthesis:** Enantioselcetive synthesis with chiral non racemic reagents and catalysts: Hydroboration with chiral boranes ($IpcBH_2$), $(Ipc)_2BH$, Carbonyl group reduction with chiral complex hydride (BINAL-H, Chiral oxazaborolidines), Chiral organometal complex–(-)DAIB; 3-exo-dimethylamino isoborneol. Enantioselective hydrogenation with [Rh(DIPAMP)]+. Diastereoselective synthesis: Aldol reactions (Chiral enolate & Achiral Aldehyde and Achiral enolate and chiral aldehyde).

3. **Conformation**: conformations of acyclic and cyclic system (3 to 6 membered rings), fused (5/5 & 6/6), Spiro and bridged bicyclo systems; stability, reactivity and mechanism; allylic strain; reactions of 5/6-membered ring containing trigonal carbon (s).

4. **Reactions & Rearrangements:** Sharpless Asymmetric epoxidation, Sommelet-Hauser rearrangement, Favorskii, rearrangements, Chichibabin reaction, Wittig reaction, Hofmann-Loffler-Freytag reaction, Barton reaction, Shapiro reaction, Curtius, Schmidt and Lossen rearrangement, Olefin metathesis.

Outcome of teaching -learning:

On Completion of this module, the learner will be able to

- Calculate optical purity and enantiomeric excess.
- Discuss the relative stability of conformational isomers of cyclohexanes and related compounds.
- Draw all the stereoisomers of organic compounds, and recognise diastereomers, enantiomers, meso compounds and centres of symmetry.
- Recognise and discuss the stereoisomers of chiral compounds that do not contain a stereogenic carbon centre and assign the configuration of the stereoisomers.
- Explain and predict the stereochemical outcome of asymmetric organic reactions for examples, hydroboration by chiral boranes, reduction of ketones by chiral boron-based reagents, asymmetric hydrogenation by using chiral catalyst etc. and their mechanism.

Books Recommended

1. M.B. Smith and J. March, March's Advanced Organic Chemistry-Reactions, Mechanisms and Structure, 5th Edition (2001), John Wiley & Sons, New York.
2. D. Nasipuri, Stereochemistry of Organic Compounds, 2nd Edition (1994), Wiley Eastern Ltd., New Delhi.
3. J. Aube and R. E. Gawley, Principles of Asymmetric Synthesis.
4. E.L. Eliel, S.H. Wilen and L.N. Mander, Stereochemistry of Organic Compounds, Wiley Interscience, New York (2004).
5. Paul de Mayo, Molecular Rearrangements, Vol.I & II, Interscience Publishers, New York (1963).
6. J. Clayden, N. Greeves, S. Warren and P. Wothers, Organic chemistry, Oxford University press INC, New York, 2001

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CMT-304(O): CHEMISTRY OF NATURAL PRODUCTS

Credits: 3

Teaching and learning: The concerned students manifest their capability of imagination and understanding by learning a specified course. They develop their ability to understand complex situations and improve their vision for taking decision.

1. **Alkaloids:** Structure elucidation of alkaloids – A general account; Structural and, Retrosynthetic analysis, synthesis and stereochemistry of Quinine and Morphine.

2. **Terpenoids:** Structure elucidation, Retrosynthetic analysis and synthesis of Camphor, and Abietic acid.

3. **Steroids:** Structure elucidation and Synthesis of Cholesterol; Synthesis of Progesterone and Aldosterone

4. **Prostaglandins:** Introduction, nomenclature of prostaglandins; approaches to prostaglandin synthesis; cyclohexane precurors (Woodward synthesis of $PGF_{2\alpha}$), bicycloheptane precursors (Corey's synthesis of prostaglandins E and F)

5. **Carbohydrates:** Conformational analysis of monosaccharides (Pentoses and hexoses); Anomeric and reverse anomeric effect; Mutarotation and abnormal mutarotation; Use of complexing agents: Borates and Phosphates; synthesis of glycosides; general treatment of polysaccharide chemistry: Hydrolysis, methylation and per-iodic oxidation, Smith degradation.

Outcome of teaching -learning:

momenta–Clabsch-Gordan series, Term symbols for two equivalent electrons, Total angular momentum and spin-orbit interaction. Condon Slater Rules.

4. **Ab initio Methods for Closed Shell Systems:** Review of molecular structure calculations, dipole moments. Hartree-Fock method for molecules. Roothaan-Hartree-Fock method. Selection of basis sets. Density functional Method. Population analysis.

Outcome of teaching -learning:

- After completion of the designed course students will be enriched with knowledge to deal microscopic world with the help of quantum chemistry.
- The concept of operator and their properties will help students to find out different observable quantity in microscopic chemical systems.
- The knowledge of various approximation methods helps course learner to evaluate the properties of many molecular systems.
- In particular the time dependent approximation methods will help to predict the spectroscopic transition in molecules.
- First principle Ab-inition calculation will help students to predict different physiochemical properties of different chemical species.

Books Recommended

1. P.W. Atkins and R.S. Friedman, *Molecular Quantum Mechanics,* 3rd edition (1997), Oxford University Press. Oxford.
2. H. Eyring, J. Walter and G.E. Kimball, *Quantum Chemistry,* John Wiley, New York (1944)
3. I.N. Levine, *Quantum Chemistry*, 5th edition (2000), Pearson Educ., Inc., New Delhi.
4. G. M. Barrow, Physical Chemistry, Fifth edition, Tata MacGraw Hill, New delhi (1994).
5. J. N. Gurtu and A. Gurtu, Advanced Physical Chemistry, Pragati Edition, Meerut (2009).

Elective Papers

Elective-I (Group A)

CMT-305: Forensic Analysis

Credits:3

Teaching and learning: To study the different aspects of forensic analysis, real case studies and forensic toxicology, applications of various instrumentation in forensic analysis.

1. **Introduction:** Profile of a forensic laboratory, Forensic Scientists role and quality control, Crime-scene investigation, Collection and preserving physical evidences and evidentiary documentation, Future prospects of forensic analysis

2. **Real Case Analysis:** Liquor analysis, Trap-case analysis, Petroleum product analysis, Fire and Debris analysis, Injuries, Firearm wounds, Asphyxia and stress analysis (only analytical identifications).

3. **Forensic Toxicology:** Analysis of various types of poisons (corrosive, irritant, analgesic, hypnotic, tranquillizer, narcotic, stimulants, paralytic, antihistamine, domestic and industrial (gaseous and volatile) poisoning and food poisonings), Explosive and explosion residue analysis, Lethal drug analysis (sampling, sealing, packing, laboratory methods of testing, reporting the analysis results, court evidence and medico-legal aspects for the consideration of chemical data as a proof for crime), Importance of physiological tests in forensic toxicology

4. **Instrumentation for Forensic Analysis**

5. **(a) *Physical, Biological and Chemical Methods:*** Non-destructive testing probes including radiography, Xera-radiography, Surface penetrations method (SEM and Laser Probes), Fluoroscopy, Clinical methods: ELISA, RIA and immunodiffusion , analysis of glucose, bilirubins, total cholesterol , creatinine, blood urea nitrogen and barbiturates in biological fluids, DNA-finger printing, Examination and grouping of blood strains and seminal strains, Data retrieval and automation techniques for forensic examination with reference to presence of drugs, glasses, paints, oils and adhesives at crime spot.

(b) *Instrumental Methods:* Sample preparation, Calibration of the instruments for its accuracy and producibility of results in forensic analysis, Method validation technique and requirements, Procurement of standard samples, Forensic applications of TLC, HPTLC, HPLC, GC, FT-IR, AAS, GC-MS, UV-visible spectrophotometer with emphasis over standard operational procedures (SOPs) for test samples.

Outcome of teaching -learning:

Student will learn about the importance of forensic analysis in real case studies and using different types of instrumental techniques.

Books Recommended

1. W.J. Welcher (Ed.), *Scott's Standard Methods of Chemical Analysis*, Vol. III A, 6th Edition (1966), and vol. III B, 5th Edition (1975), Van Nostrand Reinhold Co. London.
2. Peter Fordham, *Non-destructive Testing Techniques,* 1st edition (1968), London Business Publications Ltd., London
3. W. Horwitz, *Official Methods of Analysis*, 11th Edition (1970), Association of Official Analytical Chemists, Washington DC.
4. K. Simpson and B. Knight, *Forensic Medicine*, 9th Edition (1985), Edward Arnold Publishers Ltd., London.

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CMT-306: Chemical Applications of Group Theory

Credits: 3

Teaching and learning: To study the classification of groups, symmetry elements and point groups, Matrices and chemical applications of group theory in IR, Raman, Crystal field theory, MOT and electronic spectra.

1. **Group Theory in Chemistry:** Classification of Groups; Matrix representation of symmetry elements and point groups, matrices of C_{3v} and C_{4v} point groups, transformation matrices; Structure of character tables, determination of symmetry species for translations and rotations, Construction of Character tables (C_{2v}, C_{3v}, C_{4v} groups)

2. **Chemical Applications of Group theory**

3. **IR and Raman Spectroscopy:** Brief introduction to molecular vibrations; selection rules for fundamental vibrational transitions, symmetry of normal modes of molecules, Infrared and Raman activity of some typical molecules (molecules of C_{2v}, C_{3v}, C_{4v}, D_{2h}, D_{3h}, and D_{4h} point groups)

4. **Crystal Field Theory:** Splitting of levels and terms in chemical environment, construction of energy level diagrams, selection rules and polarizations.

5. **Molecular Orbital Theory:** Introduction, transformation properties of atomic orbitals; hybridization schemes for σ- and π-bonding, hybrid orbitals as LCAOs; Molecular Orbital Theory for some typical AB_n types (n = 2, 3, 4, 6) of molecules (H_2O, NH_3 and BH_3)

6. **Electronic Spectra:** General considerations, typical examples from tetrahedral and octahedral systems, Orgel energy level diagrams

Outcome of teaching -learning:
Student will learn about the different types of groups, Matrices, symmetry, and the application of group theory in various techniques such as IR, Raman, MOT etc.

Books Recommended

1. F. A. Cotton, *Chemical Applications of Group Theory*, 3rd Edn. (1999), John Wiley & Sons, New York.
2. G. L. Miessler and D. A. Tarr, *Inorganic Chemistry*, 2nd Edn. (1999), Prentice Hall International Inc., London.
3. K. Veera Reddy, *Symmetry and Spectroscopy of Molecules*, New Age International Pvt. Ltd., New Delhi (1999).

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CMT-307: MEDICINAL CHEMISTRY

Credits: 3

Teaching and learning: To get the knowledge of structure and activity of drugs, Antibiotics, Antimalarials, Anti-inflammatory drug etc.

1. **Structure and activity**: Relationship between chemical structure and biological activity (SAR). Receptor Site Theory. Approaches to drug design. Introduction to combinatorial synthesis in drug discovery.
2. **Few Important Drugs:**
   (a)Antibiotics and antibacterials:
   (i) Introduction
   (ii) Antibiotic β-Lactam type - Penicillins, Cephalosporins
   (iii) Anticancer - Dactinomycin (Actinomycin D), Methoxytrexate
   (iv) Antibacterial – Ciprofloxacin, Norfloxacin
   (v) Antiviral – Acyclovir
   (b) **Antimalarials:** Chemotherapy of malaria. SAR. Chloroquine, Chloroguanide and Mefloquine
   (c) **Non-steroidal and Anti-inflammatory Drugs**: Diclofenac Sodium, Ibuprofen and Netopam
   (d) **Antihistaminic and antiasthmatic agents**: Terfenadine, Cinnarizine, Salbutamol and Beclomethasone dipropionate.

Outcome of teaching -learning:

Understanding of the basic biological and pharmacological interactions by using both natural products and total synthesis of bioactive molecules. Use of corresponding knowledge for the development of biologically and clinically active drugs. It will include advanced courses in natural products, organic synthesis, medicinal chemistry; fundamentals of cell biology, molecular biology, drug design and analytical methods.

Books Recommended

1. Burger, Medicinal Chemistry, Vol. I-III, (1995) Wiley Interscience Publications, New York.
2. W. O. Foye, Principles of Medicinal Chemistry, 3rd Edition (1989), Lea & Febiger/ Varghese Publishing House, Bombay.
3. D. Lednicer and L. A. Mitscher, The Organic Chemistry of Drug Synthesis, Vol. I-III, Wiley Interscience.
4. A. Kar, Medicinal Chemistry, (1993) Wiley Eastern Ltd., New Delhi.
5. N. K. Terrett, Combinatorial Chemistry, (1998) Oxford Univ. Press, Oxford.

CMT-308: Physical Methods in Chemistry

Credits: 3

Teaching and learning: To study the principles nd applications of Photoelectron spectroscopy, AES and XRF, STM, AFM and fluorescence techniques.

1. **Photoelectron Spectroscopy and Related Techniques:** Principle and applications to studies of molecules and surface. UPES and XPS. Auger electron and X-ray fluorescence spectroscopy (AES and XRF).
2. **Techniques for Studying Surface Structure:** Low energy electron diffraction (LEED). Scanning tunneling and atomic force microscopy (STM and AFM).
3. **Neutron Diffraction:** Principle and applications.
4. **Fluorescence techniques:** Steady state fluorescence spectroscopy. Time-resolved (Time correlated single photon counting-TCSPC) fluorescence spectroscopy. Introduction to Single molecule fluorescence and fluorescence imaging.

Outcome of teaching -learning:
Student will learn about the principles and instrumentation of photoelectron spectroscopy, techniques for surface studies such as STM, AFM *etc*. Use of fluorescence techniques.

Books Recommended

1. J.M. Hollas, *Modern Spectroscopy*, 4th edition (2004), John Wiley and Sons, Chichester.
2. C.N. Banwell and E.M. Mc Cash, *Fundamentals of Molecular Spectroscopy*, 4th edition (1994), Tata McGraw Hill, New Delhi.
3. E.M. Mc Cash, *Surface Chemistry*, Oxford University Press, Oxford (2001).
4. A.K. Cheetham and P Day, *Solid State Chemistry Techniques*, Oxford Univ. Press, Oxford (1988).
5. Joseph R. Lakowicz, *Fluorescence Spectroscopy*, 2nd edition, Plenum Press, New York. (1999).

Practical

CMP-309 (A): Analytical Chemistry Practical

Credits: 6

Teaching and learning: The learners should be able to validate the conceptual understanding acquired from the theory classes

1. Solvent Extraction: Determination of Fe (III) by chloride extraction in ether
2. Determination of Cd^{2+} ions concentration in given solution by voltammetrically (i) calibration (ii) standard addition
3. Determination of Na_2CO_3 content (%) of washing soda using a pH meter
4. Estimation of carbohydrate using Anthrone method
5. Determination of nitrogen and phosphorus in soil samples
6. Determination of ascorbic acid by titration method
7. Estimation of the purity of oxalic acid employing standard Ce (IV) solution.

Outcome of teaching -learning:

- The module will provide the hands -on on different types of separation methods and

analytical instruments to prepare, separate and quantify samples from various matrices.

- Apply the scientific process, including statistical analysis of data, conducting and presenting the data of chemical analysis.
- Able to develop methods for tracing and measuring new substances, such as performance drugs.

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CMP-309(I):Inorganic Chemistry Practical ***Credits: 6***

Teaching and learning: The learners should be able to validate the conceptual understanding acquired from the theory classes

Section-A

1. (a) Synthesis and structural characterization (IR, electronic spectra and magnetic susceptibility) of $[Ni(py)_4(NCS)_2]$.

   (b) Synthesis of a series of Ni(II) complexes (with ligands of varying ligand field strength), electronic spectral interpretation and calculation of various ligand-field parameters.
2. Synthesis and structural characterization (IR, Electronic spectra) of the *cis*- and *trans*-isomers of $[Co(en)_2Cl_2]$
3. Synthesis and characterization (IR and PMR & CMR) of $[Al(acac)_3]$

Section-B

1. Synthesis, purification by sublimation and structural characterization (IR and electronic spectra) of ferrocene.
2. Acetylation of ferrocene and separation of the acetyl derivative by column chromatography.

Outcome of teaching -learning:

- Knowing about IR, electronic spectra and magnetic susceptibility of various transition metal complexes.
- Calculation of ligand field parameters based on electronic spectra of various transition metal complexes.
- Student will have idea about instrumentation methods of structural determination.

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CMP-309(O): Organic Chemistry Practical ***Credits: 6***

Teaching and learning: The learners should be able to validate the conceptual understanding acquired from the theory classes

1. Some important techniques related to organic separation: Paper Chromatography, Thin layer Chromatography, Column chromatography.
2. Estimation of Nitrogen by Kjheldal method and Sulphur by Messenger method.
3. Organic Synthesis involving 2-3 steps.

Outcome of teaching -learning:

On Completion of this module, the learner will be able to:

- Independently identify the presence of different components/molecules in the unknown

mixture

- Design a particular organic synthesis
- Purify the reaction products by various techniques such as recrystallization, TLC, column chromatography etc.

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CMP-309 (P): Physical Chemistry Practical ***Credits: 6***

Teaching and learning: The learners should be able to validate the conceptual understanding acquired from the theory classes.

1. Kinetics of decomposition of benzene diazonium chloride.
2. Conductometric study of the kinetics of saponification of ethyl acetate.
3. Determination of transport numbers of Cu^{2+} and SO_4^{2-} by Hittorf's method.
4. Conductometric titration of triple mixture (HCl+NH_4Cl+KCl) with (i) NaOH and (ii) $AgNO_3$.
5. Analysis of halide mixture by differential potentiometry.
6. Conductometric titration of a polybasic acid.
7. Verification of the Nernst law of electrode potential.
8. Ternary phase diagram of water, benzene, and acetic acid.
9. Determination of molecular weight of a macromolecule by viscometry.
10. Electrochemical Impedance study of metal/solution interface.
11. Cyclic Voltammetry of the $[Fe(CN)_6]^{3-}/[Fe(CN)_6]^{4-}$ system.
12. Corrosion study of steel in an acid solution.

Outcome of teaching -learning:

At the end of the course, the learners should be able to: Explain the principle behind the experiments performed in the laboratory Plan and Perform experiments and Interpret experimental results

Note: Experiments may be added/deleted subject to availability of time and facilities.

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Semester-IV

CMT-401: Computer Applications in Chemistry
(Core Paper)

Credits: 3

Teaching and learning: To get a brief knowledge of FORTRAN 77 and other numerical methods.

1. **FORTRAN 77:** Types of Constants and Variables in Fortran, Dimension, Data, Type, COMMON and EQUIVALENCE statements, Arithmetic and Logical IF, IF-THEN-ELSE Constructs, DO statement, Various types of I/O statements, Library functions, Statement functions, Function Subprograms and subroutine subprograms with suitable examples
2. **Numerical Methods:** Roots of Polynomials, Solution of Linear simultaneous equations,

matrix multiplication and inversion. Numerical integration. Statistical treatment of data, variance and correlations, Least square curve fitting.

Outcome of teaching -learning:

Student will learn different programming languages which are required for helping in different molecular simulations.

Books Recommended

1. V. Rajaraman, *Fortran 77*, Prentice Hall (India), New Delhi.
2. K. V. Raman, *Computers in Chemistry,* Tata McGraw Hill (1993).
3. C. Xavier, Fortran 77 and Numerical Methods, New Age International Pvt. Ltd. Publishers, New Delhi
4. S. Lipschutz and A. Poe, Schaum's Outline Series – Theory and Problems of Programming with Fortran including structured Fortran, Mc Graw Hill Book Company, Singapore

Analytical Chemistry Specialization

CMT-402(A): Advanced Separation Techniques

Credits: 3

Teaching and learning: To study about different types of separation techniques like solvent extraction, chromatography etc. A detailed knowledge of Mass spectrometry and other hyphenated techniques.

1. **Separation Techniques Based on Phase Equilibria:** Solvent Extraction: Liquid-Liquid and super critical fluid extraction, Quantitative treatment of various solvent, extraction equilibria.
2. **Separation Techniques Based on Rate Processes:** (a) Barrier-separation methods: Membrane separation-Ultrafiltration, dialysis, electrodialysis, electro-osmosis, reverse osmosis (b) Field separation methods: Electrophoresis, Ultracentrifugation.
3. **Chromatographic Separation:** Gas chromatography, high performance liquid chromatography, Ion-exchange chromatography, Reverse phase chromatography & Bonded phase chromatography (BPC), Size exclusion chromatography, Super critical fluid chromatography (SFC).
4. **Mass Spectrometry:** Principle, classification (EI, CI, FD and FAB, MALDI, SIMS and ESI) and applications in characterization of organic compounds, mass analyzers, mass spectral fragmentation of organic compounds, molecular ion peak, metastable peak and nitrogen rule.
5. **Hyphenated mass spectrometric techniques:** GC-MS, LC-MS, CE-MS, ICP-MS, tandem mass spectrometers, principle and applications.

Outcome of teaching -learning:

Student will get the knowledge (principles and instrumentation and applications) about different types of separation techniques such as solvent extraction, chromatographic separation, hyphenated mass spectrometric techniques and analysis of different samples using these techniques.

Books Recommended

1. Skoog, West, Holler & Crouch, *Fundamentals of Analytical Chemistry,* 8th Edition, Cengage Learning PVT. Ltd.

2. J.D. Seader and E.J. Henley, *Separation Process Principles*, 1st Edition (1998), John Wiley & Sons. Inc., New York.
3. Willard, Merrit, Dean, Settle, *Instrumental Methods of Analysis*, 7th Ediion, CBS Publishers & Distributors PVT Ltd.
4. G.D. Christian, *Analytical Chemistry*, John Wiley & Sons, New York (2001).
5. J. H. Gross, Mass Spectrometry: A Textbook, Springer, Verlag, Berlin, (2011).

CMT-403 (A): Electroanalytical Methods

Credits:3

Teaching and learning: To study about origin and detailed knowledge of polarography, Three electrode system, modes of electron transfer, other modern electroanalytical techniques, electroactive layers and modified electrodes.

1. **General Introduction**: Overviews of electrode processes, polarization and overvoltage, reference electrodes (Ag/AgCl, hydrogen, mercury pool) working electrodes (Pt, GCE, DME, SME, HMDE, rotating platinum electrode), Three-electrode system, factors affecting electrode reaction rate and current, Modes of mass transfer (diffusion, migration, convection).

2. **Polarography:** Ilkovic equation and its derivation, Criteria of polarographic reversibility, Interpretation of catalytic, kinetic, adsorption and capacitive currents. Polarographic maxima and maximum suppresors.

3. **Modern electroanalytical techniques:** Necessity and development of new voltammetric techniques, Oscilliography, Differential pulse voltammetry, Normal pulse voltammtery, Derivative voltammetry, Cyclic voltammetry (Reversible, irreversible, quasireversible), Linear sweep volatammetry, Alternating current voltammetry.

4. **Other related techniques:** Chronoamperometry, Chronopotentiometry. Controlled-potential and constant current coulometry, Stripping voltammetry, Electrogravimetry.

5. **Electroactive layers and modified electrodes**: chemically modified electrodes, Types, preparation and properties of films and modified electrodes: monolayers, polymers, inorganic films, biologically related materials, composites and multilayers assemblies, role of cyclic voltammetry in sensing.

Outcome of teaching -learning:

Students will learn principles, instrumentation and applications of different electroanalytical techniques, preparation methods of modified electrodes, study of different electrochemical sensors.

Books Recommended

1. *L. Meites, Polarographic Techniques, 2nd Edition (1965), John Wiley, New York.*
2. *J. Heyrovsky and K. Kuta, Principles of Polarography, 1st Edition (1966), Academic Press, New York.*
3. *D.A. Skoog, F.J. Holler and T.A. Nieman, Principles of Instrumental Analysis, 5th Edition (1998), Saunders College Publishing, Harcourt Brace & Company, U.S.A.*
4. *A.J. Bard and L.R. Faulkner, Electrochemical Methods: Fundamentals and Applications, 2nd Edition (2000), Wiley, New York.*
5. *S.Ahuja, N.Jespersen, Modern instrumental analysis, Elsevier B.V. , 2006, UK.*

Additional References

1. *C.W.C. Milner and G. Phillips, Coulometry in Analytical Chemistry, Pregamon Press, New York (1967).*

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CMT-404 (A): Instrumental Analytical Techniques

Credits: 3

Teaching and learning: To get the detailed knowledge about principle and instrumentation of IR, Raman, NMR, ESR, SEM, TEM and plasma emission spectroscopy.

1. **Infrared Spectroscopy:** Infrared instruments, typical applications of infrared spectroscopy (qualitative and quantitative).
2. **Raman Spectroscopy:** Raman spectroscopy, Instrumentation, Analytical applications of Raman spectroscopy
3. **Nuclear Magnetic Resonance Spectroscopy:** Theory of nuclear magnetic resonance, Environmental effects on NMR spectrometers, Applications of proton NMR, C13 NMR, Two dimensional Fourier-transform NMR, Magnetic resonance imaging (MRI), Quantitative applications of NMR: Drug Analysis, Molecular Weight determination.
4. **Electron Spin Resonance Spectroscopy:** Theory, Instrumentation and Important analytical applications
5. **Electron Spectroscopy:** Theory, Instrumentation and applications of Electron spectroscopy (ESCA and Auger), Scanning electron microscopy (SEM), Scanning tunnelling microscopy (STM) and Atomic force microscopy (AFM).
6. **Plasma Emission Spectroscopy:** Theory, Instrumentation and Analytical applications of inductively coupled plasma emission spectroscopy (ICPE).
7. **Applications in analysis of special materials:** Analysis of dairy products, food additives, petrochemicals (including liquid and gaseous fuels), drugs and pharmaceuticals and fertilizers.

Outcome of teaching -learning:

Student will get the knowledge of principles and instrumentation of different analytical techniques and how to do the analysis using FTIR, Raman, NMR, ESR, SEM, TEM and ICPE.

Books Recommended

1. *D.A. Skoog, F.J. Holler and T.A. Nieman, Principles of Instrumental Analysis, 5th Edition (1998), Harcourt Brace & Company, Florida.*
2. *R.L. Pecsok, L. D. Shields, T. Cairns and L.C. Mc William, Modern Methods of Chemical Analysis, 2nd Edition (1976), John Wiley, New York.*
3. *J.M. Hollas, Modern Spectroscopy, 3rd Edition (1996), John Wiley, New York.*
4. *H.A. Strobel, Chemical Instrumentation – A Systematic Approach, 2nd Edition (1973), Addison Wesley, Mass.*
5. *D.C. Garratt, the Quantitative Analysis of Drugs, 2nd Edition (1992), Chapman and Hall Ltd., London.*
6. *W. Horwitz (Editor), Official Methods of Analysis, 11th Edition (1970), Association of Official Analytical Chemists, Washington DC.*

Inorganic Chemistry Specialization

CMT-402 (I)- Structural Methods in Inorganic Chemistry

Credits: 3

Teaching and learning: A detailed study of Infrared, ESR, NMR, Mass Spectroscopy and Raman Spectroscopy. Applications in the interpretation of spectra especially in inorganic chemistry.

1. **NMR Spectroscopy**: (i) Use of Chemical shifts and spin-spin couplings for structural determination, (ii) Double resonance, and Dynamic processes in NMR, (iii) Decoupling phenomenon, Nuclear Overhauser Effect, DEPT spectra and structural applications in ^{13}C NMR, (iv) Use of Chemicals as NMR auxillary reagents (shift reagents and relaxation reagents (v) ^{1}H NMR of paramagnetic substances. (VI) NMR of Metal nuclei

2. **Electron Spin Resonance Spectroscopy**: Basic principle, Hyperfine Splitting (isotropic systems); the g-value and the factors affecting thereof; interactions affecting electron energies in paramagnetic complexes (Zero-field splitting and Kramer's degeneracy); Electron-electron interactions, Anisotropic effects (the g-value and the hyperfine couplings); Structural applications to transition metal complexes.

3. **Mössbauer Spectroscopy**: Basic principle, conditions for Mossbauer spectroscopy, Spectral parameters (Isomer shift, electric quadrupole interactions, magnetic interactions), temperature dependent effects, structural deductions for iron and tin complexes, miscellaneous applications.

4. **Infrared and Raman Spectroscopy**: Applications of vibrational spectroscopy in investigating (i) symmetry and shapes of simple AB_2, AB_3 and AB_4 molecules on the basis of spectral data, (ii) mode of bonding of ambidentate ligands (thiocyanate, nitrate, sulphate and urea).

5. **Mass Spectrometry**: Fragmentation pattern and Fingerprint applications in the interpretation of Mass spectra, effect of isotopes on the appearance of mass spectrum, recognition of the molecular ion peak; Ionization techniques (EI and FAB)

Outcome of teaching -learning:

Student will have idea about vibrational spectroscopy of different geometry metal complexes and fingerprint applications in the interpretation of mass spectra of inorganic compounds.

Books Recommended

1. *E. A. V. Ebsworth, D. W. H. Rankin and S. Cradock, Structural Methods in Inorganic Chemistry, 1st Edn.(1987), Blackwell Scientific Publications, Oxford, London.*
2. *R. S. Drago, Physical Methods in Chemistry, International Edition (1992), Affiliated East-West Press, New Delhi.*
3. *R. S. Drago, Physical Methods in Inorganic Chemistry, 1st Edn. (1971), Affiliated East-West Press, New Delhi.*
4. *K. Nakamoto, Infrared and Raman Spectra of Inorganic and Coordination Compounds, 4th Edn. (1986), John Wiley & Sons, New York.*
5. *W. Kemp, Organic Spectroscopy, 3rd Edn. (1991), Macmillan, London.*
6. *G. Aruldhas, Molecular Structure and Spectroscopy, Prentice Hall of India Pvt. Ltd., New Delhi (2001).*

CMT-403 (I): Inorganic Rings, Chains, and Clusters

Credits: 3

Teaching and learning: Metal Clusters and Metal-Metal Bonds: Compounds with metal-metal multiple bonds, metal carbonyl, halide and chalcogenide clusters. Parallels between main group

Books Recommended

1. *Jean-Marie Lehn, Supramolecular Chemistry, VCH, Weinheim (1995).*
2. *J. L. Serrano, Metallomesogens, VCH, Weinheim (1996).*
3. *Oliver Kahn, Molecular Magnetism, VCH, Weinheim (1993).*
4. *F. A. Cotton, G. Wilkinson, C. A. Murillo and M. BoCMTann, Advanced Inorganic Chemistry, 6th Edn., John Wiley & Sons (Asia) Singapore (2003).*
5. *P. Yang The Chemistry of Nanostructured Materials World Scientific Publ. Co. Pte. Ltd. (2003) ISBN 981-238-405-7.*
6. *U. Heiz and U. Landman (Eds.) Nanocatalysis, Springer, 2007.*

ORGANIC CHEMISTRY SPECIALIZATION

CMT-402(O) : Application of Spectroscopy to Structural Analysis

Credits: 3

Teaching and learning: Structure elucidation of the different organic compounds using UV, IR, PMR, CMR and Mass spectroscopy.

1 **Infrared-Ultra-Violet Spectroscopy**: UV: Absorption of dienes, polyenes, carbonyl compounds and α,β-unsaturated carbonyl compounds. Woodward rule and its application. Aromatic compounds. IR: Vibration modes and bond stretching. Absorption of common functional groups, electrical and Steric effects, effects of Hydrogen bonding. Fingerprint region and interpretation of IR spectra.

2 **PMR Spectroscopy:** Interpretation of spectra, chemical shift, shielding mechanism and anisotropic effects, chemical exchange. Spin-spin interactions, naming spin systems, magnitude of coupling constant: geminal, vicinal and long range couplings. Second order spectrum and analysis of AB, AMX and ABX systems. Simplification of Complicated Spectra: Aromatic induced shifts, spin decoupling, deuterium exchange, spectra at higher fields. Hindered rotation and rate processes.

3 **CMR Spectroscopy**: General considerations, chemical shift, coupling constants. Nuclear Overhauser effect. Spin-spin, spin-lattice relexations. Off resonance decoupling. DEPT. Interpretation of simple CMR spectra. 2 DNMR: COSY, NOESY and HETCOR.

4 **Mass Spectrometry:** Introduction, ion production, fragmentation, factors influencing ion abundance, single and multiple bond cleavage, rearrangements, cleavage associated with common functional groups, molecular ion peak, metastable ion peak, Nitrogen rule and interpretation of mass spectra.

Outcome of teaching -learning:

To learn about the Principle and applications of ultraviolet and Woodward Fisher Rule and understand the infra-red spectroscopy in organic structure determination. To know about the Nuclear magnetic resonance spectroscopy, proton chemical shift, spin-spin coupling, coupling constants and applications to organic structures ^{13}C resonance spectroscopy. To learn the Mass spectrometry and its applications including the optical rotatory dispersion and its applications. To study the concepts of Cotton effect, axial halo-ketone rule and octant rule. Student investigates the various chemical process by using a series of spectroscopic techniques. The various corner of synthetic chemistry related problem will be explained by these techniques.

Book Recommended

1. *J.R. Dyer, Application of Absorption Spectroscopy of Organic Compounds, Prentice Hall, New Delhi (1978).*

2. R.M. Silverstein and F.X. Webster, Spectroscopic Identification of Organic Compounds, 6th Edition (2003) John Wiley, New York.
3. D.H. Williams and I.F. Fleming, Spectroscopic Methods in Organic Chemistry, 4th Edition (1988), Tata-McGraw Hill, New Delhi.
4. P.Y Bruice, Organic Chemistry, 2nd Edition (1998) Prentice – Hall, New Delhi.

CMT-403(O) : Reagents and Reactions in Organic Synthesis

Credit: 3

Teaching and learning: To get the knowledge about importance of protection in organic synthesis, Use of reagents and catalysts in oxidation, reduction and other reactions. Metal ion promoted reactions.

1. **Protecting groups: Importance of protection in organic synthesis,** Hydroxy (acetate, MEM, MOM, Trityl), carbonyl (Acetal, ketal, Dithiane,) and amines (BOC, F-MOC, CBZ, Bn, Acetate etc).

2. **Reduction:** (i) Complex metal hydride reductions: $LiAlH_4$, $NaBH_4$ and DIBAL; reduction of aldehydes and ketones, stereochemistry of ketone reduction, (ii) Reduction of conjugated systems: Birch reduction, (iii) Hydroboration (iv) Miscellaneous: Tributyltin hydride, Wilkinson's catalyst.

3. **Oxidation:** (i) Oxidation with peracids: Oxidation of carbon-carbon double bonds (Sharpless epoxidation), carbonyl compounds, allylic carbon-hydrogen bonds, (ii) Oxidation with selenium dioxide and Osmium tetraoxide, (iii) Woodward and Prevost hydroxylation.

4. **Reagents and Reactions :**

(i) Advantages and limitation of Homogeneous and heterogenous process
(ii) Gilman's reagent – Lithium dimethylcuprate
(iii) Lithium diisopropylamide (LDA)
(iv) Dicyclohexyl carbodiimide (DDC)
(v) 1,3-Dithiane (Umpolung reagent)
(vi) Peterson's synthesis
(vii) Organophosphorus compounds (Wittig reaction)

5. **Metal ion Promoted Reactions:** Heck reaction, Suzuki reaction, Sonogashira reaction, Nigeshi, Stille reaction, Metathesis reaction, Water gas shift reaction (WGSR), Wacker-Smidt synthesis.

Outcome of teaching -learning:

On Completion of this module, the learner will be able to

- Take decision in selecting reagents for a particular organic synthesis
- Improve the yield of chemical reaction
- Perform direct inter-conversion of a particular functional group without protecting others
- Minimize formation of the byproducts or un-wanted molecules by choosing suitable reagents
- Synthesize important organic scaffolds via benign reaction conditions.

Books Recommended

1. H.O. House, Modern Synthetic Reactions, 2nd Edition (1972), Benjamin/Cummings Publishing Company, California.
2. L.F. Fieser and M. Fieser, Reagents for Organic Synthesis, Vol. 1-16, Wiley-Interscience, New York.

3. M.B. Smith and J. March, March's Advanced Organic Chemistry – Reactions, Mechanisms & Structure, 5th ed. (2001), Wiley-Interscience, New York.
4. M. B. Smith, Organic Synthesis, (1995) McGraw Hill Inc., New York.
5. J. Clayden, N. Greeves, S. Warren, and P. Wothers, Organic Chemistry, (2001) Oxford Univ. Press, Oxford.
6. P. R. Jenkins, Organometallic Reagents in Synthesis, (1992) Oxford Science Publ., Oxford.
7. F. A. Cotton, G. Wilkinson, C. M. Murillo and M. Bochmann, Advanced Inorganic Chemistry, 6th Edn, John Wiley and Sons, Inc., New York, 1999.
8. J. D. Atwood, Inorganic and Organometallic Reaction Mechanisms, 2nd Edn, VCH, New York, 1997.
9. G. W. Parshall, Homogeneous Catalysis, Wiley, New York, 1980.
10. C. N. Satterfield, Heterogeneous Catalysis in Practice, McGraw-Hill, New York, 1980.

CMT-404(O): Heterocycles and Vitamins

Credits: 3

Teaching and learning: To study general considerations, chemistry of condensed Indoles and Azoles, Six membered heterocyclic compounds and vitamins.

1. General Considerations: The Disconnection Approach and Retrosynthesis.
2. The chemistry of condensed Indoles, and Azoles such as Oxazoles, isoxazoles, pyrazoles, imidazoles and thiazoles,
3. Six-membered Heterocyclic compounds: Pyrimidines and purines. Structure and synthesis of Caffeine.
4. Vitamines: Structure determination and synthesis of (i) Thiamine (B1), (ii) Pyridoxine (B6) and (iii) Biotin (H).

Outcome of teaching -learning:

Heterocyclic compounds (five and six membered containg two atoms like O, N, S) and Vitamins are very interesting due to their distinct structure and the availability in medicinal drugs. So the technique of synthesis of heterocyclic compounds and vitamins is important. This course gives the quantitative ideas about the synthesis, properties and uses of such heterocyclic compounds and vitamins. This course aims at providing theoretical understanding of heterocyclic chemistry which includes various methods for ring synthesis and application of those methods for the preparation of specific groups of heterocyclic systems and vitamins. The students will be made familiar with particular properties, reactions, and applications of the most important as well as less common heterocycles and vitamins.

Book Recommended

1. I.L. Finar, Organic Chemistry, Vol. II, 5th Edition (1975 Longman Ltd., New Delhi.
2. T.L. Gilchrist, Heterocyclic Chemistry, 3rd Edition (1997) Addison-Wesley Longman Ltd., England
3. R.K. Bansal, Heterocyclic Chemistry: Syntheses,Reactions and Mechanisms, 3rd Edition (1999), New Age International, Publisher, New Delhi.
4. A.R. Katritzky and A.F. Pozharskii, Handbook of Heterocyclic Chemistry, 2nd Edition (2000), Pergamon Press, Oxford.
5. Advances in Heterocyclic Chemistry, A.R. Katritzky (Editor), Academic Press, New York.
6. Heterocyclic Compounds, A. Weissberger (Editor), Interscience, New York.

PHYSICAL CHEMISTRY SPECIALIZATION

CMT-402 (P): Statistical Mechanics

Credits: 3

Teaching and learning: To learn the laws of Thermodynamics, To learn Ensembles: Phase

Biosynthesis: terpenoids - C_5, C_{10}, C_{15}, C_{20} units; alkaloids- quinine and morpholine, steroids- cholesterol.

Molecular Recognition : Fullerenes : as host as well as guest , enzyme modeling using an artificial host frame work , cyclodextrins as esterase mimics , functionalized cyclodextrins ; chiral corands.Drug design(enzymes as targeted for drug design).

Outcomes of teaching -learning:
Student will learn enzymes and their classifications, Enzyme kinetics, Coenzyme chemistry, Biosynthesis and molecular recognition.

Books Recommended

1. A.L. Lehninger, *Principles of Biochemistry,* (1992) CBS Publishers, Delhi.
2. D. Voet, J.G. Voet & CW Pratt, *Fundamentals of Biochemistry*, (1999) John Wiley & Sons, New York.
3. H.R. Mahler and E.H. Cordes, *Biological Chemistry*, 2nd Edition, (1971) Harper and Row Pub., New York.
4. T.C. Bruice and S. Bentkovic, *Bioorganic Mechanisms*, Vol. I & II, (1966) W. A. Benjamin, New York.
5. H. Dugas and C. Penney, *Bioorganic Chemistry: A Chemical Approach to Enzyme Action*, (1981) Springer- Verlag, New York.
6. C. Walsh, *Enzymatic Reaction Mechanisms*, W.H. Freeman & Co., New York.
7. Supramolecular Chemistry by Jonathan, W. Steed and Jerry L. Atwood, John Wiley & Sons Ltd. 2000.
8. Oligonucleotides and analogues: A Practical approach. F. Eckstein. IRL Press, Oxford.
9. Methods in Molecular Biology. Vol. 20. Sudhir Agrawal. Humana Press Totowa, New Jersey.
10. Oligonucleotide Synthesis. A Practical Approach. M. J. Gait. IRL Press, Oxford.

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CMT-408: Materials Chemistry

Credits: 3

Teaching and learning: Students will learn about introduction of materials, their synthesis and characterizations, Superconductors, Non-linear and organic materials.

1. **Introduction:** Materials and their classification, Role of Chemistry in Material design.

2. **Synthesis and characterization of materials:** Preparative techniques: Ceramic methods; chemical strategies, chemical vapour deposition; preparation of nanomaterials, Langmuir-Blodgett Films. Fabrication of ordered nanostructures. Composition and purity of materials.

3. **High- Tc Oxide Superconductors:** Structural features of cuprate superconductors. 1-2-3 and 2-1-4 cuprates; structure. Normal state properties: anisotropy and temperature dependence of electrical resistance. Superconducting state: heat capacity, coherence length, relation between Tc and hole concentration in cuprates; mechanism of superconductivity in cuprates. Applications of high Tc-cuprates

4. **Organic Materials:** Conducting organics - Metals from molecules, charge transfer materials and conducting polymers. Organic superconductors. Fullerenes. Molecular ferromagnets and ferroelectrics. Liquid crystals: mesomorphic behaviour, optical properties of liquid crystals, display devices.

5. ***Non-linear materials:*** *Second and third order non-linear effects; molecular rectifiers and frequency doublers; unimolecular electronic devices. Photochromic materials; optical datastorage, memory and switches.*

Outcomes of teaching -learning:

Students will learn about the structure and characterizations of different types of materials such as Semiconductors, Organic and Non linear materials.

Books recommended:

1. *A.R. West, Solid State Chemistry and its Applications, John Wiley & Sons, Singapore (1984)*
2. *C.N R. Rao and J. Gopalkrishnan, New Directions in Solid State Chemistry, Cambridge Univ. Press (1997).*
3. *T. V. Ramakrishnan and C.N. Rao, Superconductivity Today, Wiley Eastern Ltd., New Delhi (1992).*
4. *P. Ball, Designing the Molecular World: Chemistry at the Frontier, Princeton Univ. Press, (1994).*

CMP-409: Projects

Credits : 6

Topic selection in consultation with the teacher; literature search from different reference books, scientific journals and using internet search; Bench work, typed write-up with proper tables, structures, figures and literature to be submitted; seminar lecture on this topic to be delivered in presence of all the teachers.

Teaching and Learning: The term courses also include a dissertation a research-based thesis project enhancing the students understanding.

Outcomes of learning:

- formulating and solving problems in the laboratory
- The principles and applications of modern chemical instrumentation, experimental design, and data analysis
- the underlying chemical and physical of instrumental methods of analysis, searching scientific journals and using internet search etc.
- how to work with others as part of a team to solve scientific problems
- how to communicate scientific information clearly and accurately, both in oral and in written forms
- the composition of written laboratory reports that summarize experimental procedures and the accurately present and interpret data

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