

GUJARAT UNIVERSITY

M.Sc. Chemistry Semester I and II

Revised Syllabus

Design and Structure of Choice Based Credit System

(Effective from 2020-2021)

| SEMESTER I | | | | | |
|-------------|---|-----------------------|------------|-----------|---------------|
| Course | | No. of hours per week | | | Total credits |
| Paper Code | Name | Lectures | Practicals | Total | |
| CHE 401 | Inorganic | 4 | -- | 4 | 4 |
| CHE 402 | Organic | 4 | -- | 4 | 4 |
| CHE 403 | Physical | 4 | -- | 4 | 4 |
| CHE 404 | Analytical | 4 | -- | 4 | 4 |
| CHE 405 PR | Practical (Inorganic + Organic) | -- | 7 | 7 | 4 |
| CHE 406 PR | Practical (Physical + Analytical) | -- | 7 | 7 | 4 |
| | Total | 16 | 14 | 30 | 24 |
| SEMESTER II | | | | | |
| CHE 407 | Inorganic | 4 | -- | 4 | 4 |
| CHE 408 | Organic | 4 | -- | 4 | 4 |
| CHE 409 | Physical | 4 | -- | 4 | 4 |
| CHE 410 | Analytical | 4 | -- | 4 | 4 |
| CHE 411 PR | Practical (Inorganic + Organic) | -- | 7 | 7 | 4 |
| CHE 412 PR | Practical (Physical + Analytical) | -- | 7 | 7 | 4 |
| | Total | 16 | 14 | 30 | 24 |

INDEX

| Subject | Page No. |
|--------------------------------------|----------|
| M.SC. SEMESTER I (Theory) | |
| CHE 401 Inorganic Chemistry | 3 |
| CHE 402 Organic Chemistry | 5 |
| CHE 403 Physical Chemistry | 8 |
| CHE 404 Analytical Chemistry | 10 |
| M.SC. SEMESTER I (Practical) | |
| CHE 405 PR Inorganic Chemistry | 11 |
| CHE 405 PR Organic Chemistry | 12 |
| CHE 406 PR Physical Chemistry | 13 |
| CHE 406 PR Analytical Chemistry | 14 |
| M.SC. SEMESTER II (Theory) | |
| CHE 407 Inorganic Chemistry | 15 |
| CHE 408 Organic Chemistry | 17 |
| CHE 409 Physical Chemistry | 19 |
| CHE 410 Analytical Chemistry | 21 |
| M.SC. SEMESTER II (Practical) | |
| CHE 411 PR Inorganic Chemistry | 22 |
| CHE 411 PR Organic Chemistry | 23 |
| CHE 412 PR Physical Chemistry | 24 |
| CHE 412 PR Analytical Chemistry | 25 |

Unit 1 Quantum Mechanics-I

- ☐ Commutation Relations: Angular Momentum Operators and their commutation relations; Ladder Operators and their commutation relations; Eigen Functions of the position Operator and Dirac Delta function; Projection Operators.
- ☐ Approximation method: Perturbation theory (First order and non-degenerate), application to hydrogen and helium atoms; Variation method and application to hydrogen atom.
- ☐ The Concept of tunnelling, Shape of the Barriers of tunneling.

Unit 2 Group Theory

- ☐ Matrices, Vectors and Operators: Matrix Algebra, Mathematics of matrices, Vectors, Transformation Operators
- ☐ Representation of point groups: Unit vectors as the basis for representation, Rotational vectors as the basis for representation, Position vectors as the basis for representation, Wave functions as the basis for representation
- ☐ Reducible and irreducible representations: Generated by bond vectors and by various orbitals
- ☐ Great Orthogonality Theorem and Character Table: GOT, General rules derived from GOT, Relation between reducible and irreducible representations of a point group, criteria for irreducibility, Construction of character table and notations followed, direct product representations

Unit 3 Organometallic Compounds

- ☐ Organometallic compounds of transition elements, stability of metal carbon bond in complexes
- ☐ Synthesis, uses and structure of organometallic compounds of π bonding organic ligands, 2-electron ligands, σ -allylic and acetylinic complexes, compound with 3 electron ligand – allylic complexes, compounds. With 4-electron ligands butadiene complexes, n^4 complexes of cyclopentadiene, compounds with 5 electron ligands–cyclopentadienyl, compounds with 6 electron ligands, n^6 complexes of benzene and its derivatives
- ☐ Role of organometallic compounds in catalytic reaction

Unit 4 Electronic Spectroscopy

- ☞ Concept of crystal field theory (CFT), ligand field theory (LFT) and molecular orbital theory (MOT);
- ☞ Splitting of d-orbitals in various stereochemistry; tetragonal distortion in octahedral complexes;
- ☞ Spectrochemical series; nephelauxetic series; electronic states and term symbols; microstates; derivation of terms for closed subshell; derivation of terms for p^2 , d^2 and f^2 configurations

REFERENCES

1. *Introductory Quantum Chemistry, Fourth Edition*, By: A. K. Chandra Tata McGraw-Hill Publishing Company Ltd., New Delhi (1994).
2. *Molecular Quantum Mechanics*, By: P. W. Atkins and R. S. Friedman Oxford University Press (1997).
3. *An Introduction to Quantum Chemistry*, By: M. Satake, Y. Mido, H. Yasuhisa, S. Taguchi, M. S. Sethi & S. A. Iqbal Discovery Publishing House New Delhi (1996).
4. *Quantum Chemistry* By: N. Levine, Prentice Hall of India (p) Ltd. New Delhi (1994).
5. *Quantum Chemistry through problem and solutions* By: R. K. Prasad New Age International Publishers (1997).
6. *Introduction to Magnetochemistry*, By: Alan Earshaw (1968)
7. *Elements of Magnetochemistry*, By: Dutta and Syamal (1993)
8. *Modern Aspects of Inorganic Chemistry*, By: Emeleus and Sharpe (1996)
9. *Advanced Inorganic Chemistry*, By: Cotton, Wilkinson, Murillo and Bochmann (1999)
10. *Inorganic Chemistry*, By: A.G. Sharpe (1981)
11. *Inorganic Chemistry*, By: James E. Huheey, Eilen A. Keiter, Richard L. Keiter Publication: Harper Collins
12. *Essentials of Coordination Chemistry: A simplified approach with 3d visuals*, Vasishta Bhatt, Academic Press, Elsevier London, 2016.
13. *Inorganic Chemistry*, By: Shriver and Atkins
14. *Inorganic Chemistry*, By: Gary Wulfsberg
15. *Descriptive Inorganic Chemistry (Fourth Edition)* By Geoff Rayner- Canham, Tina Overton Publication: Craig Bleyer
16. F. A. Cotton, *Chemical Applications of Group theory*, Wiley Eastern 3rd edition
17. George Davidson, *Group Theory for Chemists*, Macmillan Physical Science, 1991
18. *Chemical Applications of Molecular Symmetry and Group Theory*, B.S. Garg, Macmillan Publisher India Ltd (2012)
19. *Organometallic Chemistry a Unified Approach* by R.C.Mehrotra and A.Singh,
20. *Organometallic Chemistry of Transition Metals* by Robert H.Crabtree.
21. *Symmetry and Group Theory in Chemistry* by Rameshwar Ameta, 2nd edition, New Age International Publishers
22. *Molecular Structure and Symmetry* by K Veera Reddy, 1st edition, New Age International Publishers

Unit 1 Elimination, Nucleophilic and Electrophilic Substitution Reaction

- ☐ Mechanism, Orientation and stereochemistry of E1, E2 and E1CB reaction.
- ☐ Reactivity: effects of substrate structures, attacking base, solvent and leaving group
- ☐ Mechanism and orientation in pyrolytic *syn* eliminations- Chugaev, Cope elimination, Burgess Dehydration Reaction, Selenoxide Elimination and Grieco Elimination.
- ☐ Nucleophilic substitution at the carbonyl (C=O), alcohol and nitrogen: Baeyer-Villiger oxidation and the benzoin condensation, Alcohols: The Mitsunobu reaction, Nitrogen: The von Richter and Smiles rearrangements respectively.
- ☐ Neighbouring group Participation in Nucleophilic substitution: O (COO⁻, -OH), N (NH₂, NHR, NR₂), S (SH, SR), and halogen as Neighbouring group donor.
- ☐ Aromatic electrophilic substitution reactions: The arenium ion mechanism, orientation and reactivity: Vilsmeier-Hack reaction and Gattermann-Koch reaction.

Unit 2 (A) Aromaticity

- ☐ Introduction
- ☐ Huckel's rule and concept of aromaticity
- ☐ Types of aromaticity- Aromatic, Anti-aromatic, Non-aromatic
- ☐ Frost circle diagram for cyclobutadiene, benzene, etc.
- ☐ Aromaticity in benzenoid and non-benzenoid compounds and charged rings, annulenes, fulvenes, azulenes, antiaromaticity and homoaromaticity.

(B) Computer in Chemistry

- ☐ Introduction,
- ☐ Software, uses of microsoft office (Word, PPT, Excel),
- ☐ Drawing of structure, calculations of properties,
- ☐ Computer tools used in chemistry, search engines, Journals, database, literature review

Unit 3 (A) Reactive Intermediates and Rearrangements

Discuss stability, structure, generation and fate for mentioned intermediates

- ☐ Carbocations
- ☐ Carbanions
- ☐ Carbenes
- ☐ Free radicals
- ☐ Nitrene

(B) Rearrangements

General mechanistic considerations, nature of migration, migratory aptitude, and memory effects in respect of following rearrangements:

- ☐ Carbon to Carbon migration of R, H and Ar
 - a) Favorskii rearrangement
 - b) Wagner–Meerwein rearrangement
- ☐ Carbon to Nitrogen migrations:
 - a) Schmidt rearrangement
 - b) Lossen rearrangement
- ☐ Migration from Nitrogen to Carbon
 - a) Stevens rearrangement
- ☐ Migration from Oxygen to Carbon
 - a) Wittig rearrangement
 - b) Fries rearrangement

Unit 4 Stereochemistry

Introductory/Pre-requisite [*Identifying stereochemical terms & relationships (Stereochemistry, Enantiomers, Diastereomers, Conformations, Configurations, Epimers, Anomers, Prochiral, Chiral carbon, Chiral molecules, Meso, Optical activity, Specific rotation, Atrop isomerism), 2-D representations (line drawings, Fischer projections, Haworth projections) and Nomenclature (R/S, E/Z, D/L, d/l, Cis/Trans, Threo/Erythro)*]

- ☐ Determination of relative/absolute configuration and resolution by Chiral GC, HPLC
- ☐ Physical and chemical properties of stereoisomer
- ☐ Prochiral environments (enantiotopic, diastereotopic)
- ☐ Stereochemistry in SN2 (inversion),
- ☐ Stereochemistry in elimination reaction mechanisms (E2, Hoffmann)
- ☐ Stereochemistry in additions to alkenes (syn, anti, Diels-Alder)

- 📄 Stereochemistry in additions to carbonyls (Cram's rule)
- 📄 Chiral drugs,
- 📄 Stereospecific and stereoselective reaction

REFERENCES

1. *Advanced Organic Chemistry, Reactions Mechanisms and Structure*, J. March, 6th Edition, John Wiley.
2. *Carbenes, nitrenes and arynes*, T.L. Gilchrist and C.W. Rees.
3. *Reaction Mechanism in Organic Chemistry* by S. M. Mukherji and S. P. Singh
4. *Advanced Organic Chemistry Part A: Structure and Mechanism and Part B: Reaction and synthesis*, Francis A. Carey, Richard J. Sundberg, 5th Edition, Springer.
5. *Organic Chemistry*, Jonathan Clayden, Nick Greeves, Stuart Warren, 1st Edition, Oxford University Press.
6. *Reaction mechanism* by Jagdamba Singh.
7. *Organic chemistry - Reaction mechanism*, by P.S. Kalsi, New age international publishers.
8. *Reagents in Organic Synthesis- Fieser and Fieser*, John Wiley.
9. *Organic Chemistry*, T.W. Graham Solomons and Graig B. Frymes, John Wiley and Sons.
10. *Organic Chemistry*, F. A. Carey, McGraw Hill Edition.
11. *General Organic Chemistry Sachin Kumar Ghose*, New Central book agency.
12. *Organic Chemistry Vol 1-2 I.L. Finar 6th edition*, ELBS.
13. *Organic Chemistry (3/e)* by J. B. Hendrickson, Donald J. Cram and George S. Rammond
14. *Stereochemistry of organic chemistry* D. Nesh, New age publication.
15. *Basic stereochemistry of organic molecule* by Subrata.
16. <https://www.capterra.com/chemical-software/>
17. K.V. Raman, *Computers in Chemistry*, Tata McGraw-Hill Ltd., New Delhi, 1993.
18. Gini Courter and Annette Marquis, *Microsoft Office 2000*, BPB Publications, New Delhi, 1999.
19. Julia Kelly, *Using Microsoft Excel 2000*, Prentice-Hall of India, New Delhi, 1999.
20. Robert de Lavie, *A spreadsheet workbook for Quantitative chemical analysis*, McGraw-Hill, Inc. New Delhi, 1997.
21. R.P. Soni, Harshal A. Arolkar, Sonal Jain, *Working with Personal Computer Software*, 2nd Edition, Wiley India, August 2010. ISBN13: 978-81-265-2727-4.

Unit 1 Chemical Thermodynamics

- ☞ Nernst heat theorem and its applications to gaseous system,
- ☞ Third law of thermodynamics and its applications to evaluate absolute entropies of solids, liquids and gases and for calculations of free energy changes and equilibrium constants of reactions,
- ☞ Chemical affinity and its applications, methods for determining the chemical affinity of a reaction-Gibbs Helmholtz equation, E.M.F. Method, Van't Hoff equation, Vapour pressure method,
- ☞ Partial molar quantities and their determination by direct method, apparent molar properties, method of intercepts,
- ☞ Chemical potential and its physical significance, variation of chemical potential with temperature and pressure, chemical potential of ideal gases and solutions.

Unit 2 Chemical Kinetics

- ☞ Introduction, Theories of reaction rates: The collision theory of reaction rates, The transition state theory of reaction rates and its limitations, activated complex theory in terms of thermodynamic terms, elementary reactions in solutions, influence of solvent properties on rate, different types of molecular interactions in solutions, diffusion and activation controlled reactions, transmission coefficient, reaction coordinates, potential energy surfaces, kinetic isotope effect.

Unit 3 Surface Chemistry

- ☞ Physical and chemical adsorption, Special features of chemisorption-kinetics of chemisorption and heat of chemisorption, BET theory for multilayer adsorption, Experimental methods of determining gas adsorption-Volumetric and gravimetric method, Determination of surface area of adsorbents by HJ method, Benton and white method and BET Method, Gibbs adsorption isotherm equation, Experimental results of the Gibbs equation, verification of the Gibbs equation- Domain and Barker Method The Microtome method of McBain, The tracer method.

Unit 4 Solid State Chemistry

- ☰ Properties of solids – electrical, magnetic, optical, dielectric properties. Band theory of solids and energy band theory of conductors, semiconductors and insulators, Defects in crystals, calculation of Schottky and Frenkel defects using statistical method, Non stoichiometry, Solid electrolytes, diffusion in solids, electrical conductivity in solids, Super conductivity, perovskites. Determination of lattice parameters of a unit cell of NaCl crystal, Graphical method of indexing, Determination of particle size of crystallites, single crystal and phase determination method

REFERENCES

1. *Textbook of physical chemistry – W.J.Moore*
2. *Textbook of physical chemistry – Glasstone*
3. *Textbook of physical chemistry – P.Atkins*
4. *Advanced physical chemistry – Gurdeep Raj*
5. *Advanced physical chemistry – J.N.Gurtu, A.Gurtu*
6. *Thermodynamics for chemists –Glasstone*
7. *Physical chemistry – S. Castellian*
8. *Thermodynamics of non equilibrium processes- Karapitaneh*
9. *Chemical Kinetics- Laidler*
10. *Chemical Kinetics – Frost and Pearson*
11. *Solid state chemistry – H.Keer*
12. *Solid state chemistry- Hannay*
13. *Chemistry of solids – Azaroff*
14. *Surface chemistry – Adamson*
15. *Surface chemistry – Osipov*

Unit 1 Concepts and Tools of Analytical Chemistry

- Introduction, scope of analytical science and its literature, features and classification of analytical methods, basics of classical and instrumental methods of analysis, significant figures, SI units, chemical concentrations (weight %, volume %, weight-to-volume %, molarity, formality, molality, ppm, normality), unit conversions, reference standard, preparation of standard solution and standardization, dilution, stoichiometry calculations, calibration of glass apparatus
- Non-aqueous titrations: Principles, theory, role of solvents and their classification, properties of solvents, titration of acids-bases, standard titration curves, factors affecting non-aqueous titrations, advantages and limitations.

Unit 2 Data Handling and Statistical Analysis

- Measurement of uncertainty, Accuracy and precision, types of errors and their causes; Gaussian distribution, control charts, confidence limit, test of significance, rejection of a result- Q-test and Grubb's test. Finding the best straight line-least square regression, calibration curves, correlation coefficient; standard addition technique and use of internal standards, Analysis of variance, GLP-standard operating procedures, quality assurance and quality control, validation of analytical methods.

Unit 3 pH metry and Conductometry

- pH measurement with glass electrode, working of glass electrode, mechanism of pH measurement (boundary potential and diffusion potential), calibration of glass electrode, acid and alkaline errors in pH measurement. Fundamental concepts of conductometry, measurement of conductivity, apparatus, and basis of conductometric titrations-acid-base, precipitation and complex formation. High frequency titrations.

Unit 4 Potentiometry and Ion-selective Electrodes

- ☰ Electrochemical cell, cell potentials, sign convention for electrode potentials, types of reference and indicator electrodes-metallic indicator and membrane indicator electrodes, Classification of membrane electrodes-ion-selective and molecular-selective electrodes, Principle, properties and design of ion-selective electrodes, Crystalline and non-crystalline membrane electrodes, Gas-sensing probes and enzyme substrate electrodes, Applications of potentiometric titrations

REFERENCES

1. *Introductory I. "Quantitative Chemical Analysis" by Daniel C. Harris, 7th Edition, W.H. Freeman and Company, New York, 2007.*
2. *"Analytical Chemistry" by Gary D. Christian, Purnendu K. (Sandy) Dasgupta and Kevin A. Schug, 7th Edition, John Wiley and Sons Inc. New Jersey, 2014.*
3. *"Fundamental of Analytical Chemistry" by Douglas A. Skoog, Donald M. West, F. James Holler, Stanley R. Crouch, 8rd Edition, Thomson, Brookes/Cole, 2004.*
4. *"Modern Analytical Chemistry" by David Harvey, McGraw Hill, New York, 2001.*

M.SC. SEMESTER I PRACTICALS

CHE 405 PR INORGANIC CHEMISTRY (Minimum 9)

- ☰ Semi-micro qualitative analysis of 15 mixtures, each having six radicals plus one less familiar elements and one insoluble compounds.

REFERENCES

1. *Vogel's Qualitative Inorganic Analysis by G. Svehla, 7th Edition, Pearson*
2. *Inorganic Qualitative Analysis in the Laboratory, Clyde Metz, Elsevier, 2012, ISBN : 978032316104*

M.SC. SEMESTER I PRACTICALS

CHE 405 PR ORGANIC CHEMISTRY (Minimum 9)

- ☞ One step preparation of organic compounds and study of principle, general reaction mechanism, mole ratio calculation, purification, M.P/B.P and TLC.
- ☞ Distribution of Marks as per University exam: Principle and reaction mechanism (05 marks), Mole ratio and other calculation (05 marks), Crude and Crystal (10 marks), Purification, and M.P/B.P (05 marks), TLC (05 marks) and Viva (05 marks), Total 35 marks
- ☞ List of Preparations
 1. Nitration
 - a) *m*-dinitro benzene from nitro benzene
 - b) *p*-Nitro acetanilide from Acetanilide
 2. Bromination
 - a) *p*-bromo acetanilide
 - b) 2,4,6-tribromo aniline
 3. Acylation
 - a) Acetanilide from aniline
 - b) Resacetophenone from resorcinol
 4. Reduction
 - a) Preparation of *m*-nitro aniline from *m*-dinitro benzene
 - b) Preparation of *m*-phenylenediamine from *m*-dinitrobenzene
 5. Oxidation
 - a) Preparation of benzoic acid from benzaldehyde
 - b) Preparation of *p*-nitrobenzoic acid from *p*-nitro toluene (Continued.....)
 6. Condensation reaction
 - a) Preparation of dibenzal acetone from benzaldehyde
 - b) Preparation of 7-hydroxy 4-methylcoumarin
 7. Diazotization reaction
 - a) Preparation methyl orange
 - b) Preparation of methyl red
 8. Friedl-Craft's reaction
 - a) 4-methyl benzophenone (Friedal Craft reaction)
 - b) Preparation of aspirin

REFERENCES

1. *A text book of practical organic chemistry – A. I. Vogel*
2. *Practical organic Chemistry – Mann and Saunders*

M.SC. SEMESTER I PRACTICALS

CHE 406 PR PHYSICAL CHEMISTRY (Minimum 9)



Conductometry

1. To determine the thermodynamic dissociation constant of a weak acid.
2. Verification of Ostwald's dilution law and determination of the dissociation constant of a weak monobasic acid conductometrically.
3. To estimate conductometrically the quantities of HCl and NH₄ Cl in a given mixture.



Potentiometry

1. To determine the standard redox potential and the number of electrons involved in Fe⁺²/ Fe⁺³ system.
2. To determine the dissociation constant of a dibasic acids oxalic acid or malonic acid.
3. To determine the solubility product of sparingly soluble salts e.g. AgCl, AgBr and AgI



pH metry

1. To determine the dissociation constant of a polybasic acid e.g. phosphoric acid.
2. To determine the % purity of Na₂CO₃ and NaHCO₃ in the given mixture.



Chemical Kinetics and Adsorption

1. To study the effect of ionic strength of ions on the kinetics of the reaction $S_2O_8^{2-} + 2I^- \longrightarrow 2SO_4^{2-} + I_2$
2. To determine the temperature coefficient and energy of activation of reaction between K₂S₂O₈ + KI.
3. To determine the order of reaction between K₂S₂O₈ + KI by fractional change method.
4. To determine the temperature coefficient and energy of activation of hydrolysis of methyl acetate catalyzed by HCl.
5. To determine the partial molar volume and the excess volume of the binary mixtures of ethanol-water system.

REFERENCES

1. *Practical physical chemistry – J.B.Yadav*
2. *Practicals in physical chemistry – P.S.Sindhu*
3. *Experimental physical chemistry – R.C.Das, B.Behera*
4. *Experiments in physical chemistry- P.H.Parsania, F. Karia*
5. *Experimental physical chemistry – V.D. Athawale, ParulMathur*
6. *Advanced physical chemistry experiments – Gurtu-and Gurtu*

M.SC. SEMESTER I PRACTICALS

CHE 406 PR ANALYTICAL CHEMISTRY (Minimum 10)

1. Calibration of glass wares, balance, pH meter, conductometer, potentiometer and spectrophotometer.
2. Preparation of stock solutions and their standardization (HCl with NaOH, and NaOH with KHP)
3. Determination of nicotine in tobacco (non-aqueous titration).
4. Determination of available chlorine in bleaching powder.
5. Determination of vitamin C in orange juice/amla.
6. Determination of acetic acid in vinegar.
7. Determination of sodium carbonate and sodium bicarbonate in washing soda.
8. Determination of ascorbic acid in vitamin C tablets.
9. Determination of calcium and magnesium in water sample.
10. Determination of total dissolved solids in water samples.
11. Determination of sulphate in water sample.
12. Determination of chloride in water sample.
13. To determine the % of nitrogen in urea by Kjeldahl's method.
14. To determine % purity of given alcohol sample by iodometric titration.
15. Determination of fat content of milk sample.

REFERENCES

1. *Analytical Chemistry: Practice, Second Edition, John H. Kennedy, Saunders College Publishing.*
2. *Vogel's Textbook of Quantitative Chemical Analysis, Fifth edition, Longman Scientific and Technical and John Wiley & Sons, Inc., New York.*

M.SC. SEMESTER II

CHE 407 INORGANIC CHEMISTRY

Unit 1 Theories of Bonding

- ☐ VSEPR, Walsh diagram for tri-atomic molecules, Bent rule and energies of hybridization, VSIP.
- ☐ Simple Huckel theory of linear conjugated systems, cyclic conjugated systems aromaticity.
- ☐ Many electron atoms and angular momenta: The Wave function of many electron systems, application to helium atom, Hartree Self-Consistent field method. Pariser-Parr-Pople approximation.

Unit 2 Applications of Symmetry

- ☐ Molecular spectroscopy and Vibrational spectroscopy: Reducible representation using $3N$ vectors as the basis, symmetry selection rules for IR and Raman spectroscopy,
- ☐ Classification of vibrational modes using internal coordinates as the basis and assignment of frequency to fundamentals.
- ☐ Molecular symmetry and chemical bonding: hybrid orbitals for σ -bonding and π -bonding in AB_n type of molecules.
- ☐ Symmetry Adopted Linear Combination of Atomic orbitals: Projection operator for finding SALC, Bond vectors as the basis for formation of SALC, Orbital functions as the basis for obtaining SALC.

Unit 3 Bioinorganic Chemistry

- ☐ Hemoglobin and Myoglobin; Cytochromes of the electron transport chain, Cytochrome P-450 enzymes, Coenzyme B12, Zinc Enzymes exploiting acid catalysis: Carbonic anhydrase, Carboxy peptidases, Biological Nitrogen Fixation, The elements of living system: The biological roles of metal ions
- ☐ **Metals in medicine:** Chelation Therapy, gold in Rheumatoid antiarthritis drugs, Metallocenes, Anticancer agents- Platinum complexes, mechanism of action, aspects of Pt binding to DNA, Metal complexes as radiodiagnostic agents, Magnetic resonance imaging
- ☐ **Metal-nucleic acid interactions:** Coordination, Non-covalent interactions - intercalation and hydrogen bonding, hydrophobic interactions, DNA strand cleavage, Biological fluorophores, Application of fluorescence quenching in drug-DNA binding studies. DNA binding and mechanistic possibility

Unit 4 Metal-Ligand Equilibria

- Types of Complex Equilibria in Solution and Equilibrium Constants: Basic principles, Mathematical functions and their interrelationship. Statistical considerations. Factors affecting the stability constants of Metal complexes. Mixed-ligand complexes.
- Experimental Methods for the Determination of Stability Constants:** Ion exchange methods, Polarographic methods. Solubility methods and Least square method for computing stability constant.

REFERENCES

1. *Introductory Quantum Chemistry, Fourth Edition, By: A. K. Chandra Tata McGraw-Hill Publishing Company Ltd., New Delhi (1994).*
2. *Molecular Quantum Mechanics, By: P. W. Atkins and R. S. Friedman Oxford University Press (1997).*
3. *An Introduction to Quantum Chemistry, By: M. Satake, Y. Mido, H. Yasuhisa, S. Taguchi, M. S. Sethi & S. A. Iqbal Discovery Publishing House New Delhi (1996).*
4. *Quantum Chemistry By: N. Levine, Prentice Hall of India (p) Ltd. New Delhi (1994).*
5. *Quantum Chemistry through problem and solutions By: R. K. Prasad New Age International Publishers (1997).*
6. *Introduction to Magnetochemistry, By: Alan Earshaw (1968)*
7. *Elements of Magnetochemistry, By: Dutta and Syamal (1993)*
8. *Modern Aspects of Inorganic Chemistry, By: Emeleus and Sharpe (1996)*
9. *Advanced Inorganic Chemistry, By: Cotton, Wilkinson, Murillo and Bochmann (1999)*
10. *Inorganic Chemistry, By: A.G. Sharpe (1981)*
11. *Inorganic Chemistry, By: James E. Huheey, Eilen A. Keiter, Richard L. Keiter Publication: Harper Collins*
12. *Essentials of Coordination Chemistry: A simplified approach with 3d visuals, Vasishta Bhatt, Academic Press, Elsevier London, 2016.*
13. *Inorganic Chemistry, By: Shriver and Atkins*
14. *Inorganic Chemistry, By: Gary Wulfsberg*
15. *Descriptive Inorganic Chemistry (Fourth Edition) By Geoff Rayner- Canham, Tina Overton Publication: Craig Bleyer*
16. *F. A. Cotton, Chemical Applications of Group theory, Wiley Eastern 2nd Edn. 1992*
17. *George Davidson, Group Theory for Chemists, Macmillan Physical Science, 1991*
18. *Chemical Applications of Molecular Symmetry and Group Theory, B.S. Garg, Macmillan Publisher India Ltd (2012)*
19. *Symmetry and Group Theory in Chemistry by Rameshwar Ameta, 2nd edition, New Age International Publishers*
20. *Molecular Structure and Symmetry by K Veera Reddy, 1st edition, New Age International Publishers*

M.SC. SEMESTER II

CHE 408 ORGANIC CHEMISTRY


Unit 1 Photochemistry

1. Mechanism, Photochemical reactions: Principles of energy transfer, electronic excitation
2. Characteristics of photochemical reactions
3. Jablonski diagram
4. Chemiluminescence, Bioluminescence
5. Photosensitization
6. Photochemistry of carbonyl compounds: Representation of excited states of ketones
7. Photoreduction
8. Norrish type I & II reactions, Reactions of cyclic Ketone and acyclic Ketone
9. Oxetane formation (Paterno-Buchi reaction)
10. Di- π methane rearrangement
11. cis-trans isomerisation
12. Photo-Fries rearrangement
13. Applications of photochemistry

Unit 2 Heterocyclic Compounds

1. Introduction
2. Nomenclature of Heterocyclic compounds
3. Pyridine conceptually derived from Benzene, replacing CH with N
4. Pyrrole derived from benzene, replacing CH=CH with N
5. Reactions of Pyridine and its derivatives
6. Reactions of Pyrrole and its derivatives
7. Comparison of Pyrrole with furan and thiophene
8. Chemistry of Imidazole, Triazoles, Tetrazole
9. Fused rings: indole, quinoline, isoquinoline, and indolizine
10. Chemistry of Oxazole, Thiazole, Isoxazole, Isothiazole
11. Importance of heterocyclic compounds in medicinal chemistry

Unit 3 Name Reactions

-  Total 10 name reactions and their principle, general reaction, mechanism, synthetic application, advantages, disadvantages and modification-scope of reaction,

1. Suzuki reaction
2. Sonogashira coupling
3. Buchwald-Hartwig reaction
4. Knoevenagel reaction
5. Shapiro reaction
6. Ugi reaction
7. Biginelli reaction
8. Nazarov cyclization
9. Ullmann reaction.
10. Baylis-Hilman

Unit 4 Reagents in organic synthesis

 Total 10 reagents, mechanism, selectivity and utility of following reagents:

1. HATU
2. Lithium diisopropylamide (LDA)
3. Dicyclohexyl carbodiimide (DCC)
4. 1,3 – Dithiane (Umpolung reagent)
5. Dess- Martin periodinane
6. Diisobutylaluminum hydride (DIBAL-H)
7. Sodium cyanoborohydride (NaBH₃CN)
8. DDQ
9. n-Butyl lithium
10. Phase transfer catalysis : Quaternary ammonium and phosphonium salts, crown ethers.

REFERENCES

1. *Advanced Spectrometric Identification of Organic Compounds* by Robert M. Silverstein, 7th Edition
2. *Introductory Photochemistry*, A.Cox and T.Camp, McGraw Hill.
3. *Photochemistry*, R.P. Kundall and A. Gilbert, Thomson Nelson.
4. *Organic Photochemistry*, J. Coxon and B. Halton, 2nd Edition , Cambridge University Press.
5. *Strategic Applications of Named Reactions in Organic Synthesis*, Laszlo Kurti and Barbara Czak, 1st Edition , Academic Press.
6. *Name Reactions and Reagents in Organic Synthesis*, Bradford P. Mundy, Michael G. Eller, Frank G. Favalaro, 2nd Edition, Wiley – Interscience.
7. *Name Reactions. A Collection of Detailed Reaction Mechanisms.*, Jie Jack Li, 3rd Edition , Springer.
8. *Heterocyclic Chemistry, volume 1-3*, R.R. Gupta, M. Kumar and V. Gupta, Springer-Verlag.
9. *Heterocyclic Chemistry*, J.A. Joule, K.Mills, and G.F. Smith, 3rd Edition, Chapman and Hall.

10. *Heterocyclic Chemistry*, T.L. Gilchrist, Longman Scientific Technical.
11. *Contemporary Heterocyclic Chemistry*, G.R. Nikome and W.W. Poudler, Wiley.
12. *Comprehensive Heterocyclic Chemistry*, A.R. Kartizky, and C.W. Rees.
13. *Encyclopedia of Reagents for Organic Synthesis*, Leo A. Paquette, David Crich and Phillip L. Fuchs, John Wiley and Sons Inc.
14. *Organic Chemistry*, T.W. Graham Solomons and Graig B. Frymes, John Wiley and Sons.
15. *Organic Chemistry*, F. A. Carey, McGraw Hill Edition.
16. *General Organic Chemistry Sachin Kumar Ghose*, New Central book agency.
17. *Guidebook to Mechanism in Organic Chemistry by Peter Sykes*, 6th Edition, Prentice Hall.
18. *Advanced Organic Chemistry Part A: Structure and Mechanism and Part B: Reaction and synthesis*, Francis A. Carey, Richard J. Sundberg, 5th Edition, Springer.
19. *Organic Chemistry Vol 1-2 I.L.Finar* 6th edition, ELBS.
20. *Name Reactions and Reagents in Organic Synthesis By Bradford P. Mundy, Michael G. Eller, Frank G. Favaloro.*
21. *Organic Syntheses Based on Name Reactions: By Alfred Hassner, Irishi Namboothiri.*

M.SC. SEMESTER II

CHE 409 PHYSICAL CHEMISTRY

Unit 1 Statistical Thermodynamics

- ☰ Concepts of distribution of molecules, thermodynamic probability, permutations and combinations, The Boltzmann distribution law, relationship between molecular partition function and thermodynamic function thermodynamic properties in terms of molar partition function Partition function - translational, vibrational, rotational, electronic nuclear partition functions separation of partition function of polyatomic molecules. Bose-Einstein statistics, Fermi-Dirac statistics.

Unit 2 Polymer Chemistry

- ☰ Introduction, mechanism and kinetics of polymer processes, criteria of polymer solubility, thermodynamic of polymer solution, F-H theory, polymer analysis and characterization- identification, physical testing method – thermal and chemical, characterization-molecular weight distribution, determination of molecular weight of polymers, glass transition temperature, factors affecting glass transition temperature, glass transition temperature and molecular weight, Importance of glass transition temperature.

Unit 3 Nuclear and Radio Chemistry

- ☰ Nuclear properties-nuclear radius, coulombic and nuclear potential radius, nuclear binding energy, nuclear models-shell model, liquid drop model, radioactive decay nuclear reactions, evaporation, spallation, fragmentation, fission and fusion reactions, Reaction cross section, Use of radioisotopes as tracers: Reaction mechanism, Structure determination, Isotope dilution analysis: (i) Direct Isotope dilution analysis (DIDA), (ii) Inverse Isotope Dilution Analysis (IIDA), and (iii) Sub stoichiometric isotope dilution analysis, Dating ¹⁴C, Medical applications.

Unit 4 Electrochemistry

- ☰ Basic concepts: Determination of dissociation constant of monobasic acids by conductometry, Determination of dissociation constants of monobasic and polybasic acids by potentiometry, The electrical double layer, the rate of charge transfer, Determination of activities of solutes from activities of solvent, Dependence of electrolyte activity on hydration number, Bjerrum's theory of ion association in electrolyte solutions, Determination of interfacial tension of mercury as a function of potential across the interface.

REFERENCES

1. *Textbook of physical chemistry – W.J.Moore*
2. *Textbook of physical chemistry – Glasstone*
3. *Textbook of physical chemistry – P.Atkins*
4. *Advanced physical chemistry – Surdeep Raj*
5. *Advanced physical chemistry – J.N.Gurtu, A.Gurtu*
6. *Statistical thermodynamics – M.C.Gupta*
7. *Polymer chemistry – Gowariker*
8. *Polymer chemistry – Billmayer*
9. *Principles of polymer science – Bahadur & Sastry*
10. *Polymer science & technology – Fried*
11. *Polymer chemistry- Malcolm P. Stevens*
12. *Nuclear chemistry – Arniker*
13. *Nuclear and radio chemistry – J.W. Kannedy, G.Friedlander*
14. *Electrochemistry – Bockris and Reddy*

Unit 1 Sampling and Sample Preparation Techniques

- ☰ Sampling and sample preparation, general steps in chemical analysis, Liquid-liquid extraction/solvent extraction-partition coefficient, distribution ratio and percent extraction. Solvent extraction of metal ions-ion association complexes and metal chelates, multiple batch extraction, Craig's counter-current distribution, Cloud point extraction, Accelerated and Microwave assisted extraction, protein precipitation and solid phase extraction (SPE), Hybrid SPE and solid phase micro extraction (SPME).

Unit 2 Chromatographic Methods

- ☰ Principles of chromatography, classification of chromatographic techniques based on mechanism of retention, configuration, mobile and stationary phase, Efficiency of separation- plate theory (theoretical plate concept) and rate theory (Van Deemter equation), Principles and applications of thin layer chromatography (TLC), high performance thin layer chromatography (HPTLC), ion exchange chromatography, and ion-chromatography and high performance liquid chromatography (HPLC).

Unit 3 Spectrophotometry

- ☰ Properties of light, absorption of light, interaction of light with matter and origin of spectra, The spectrophotometer- calibration, sources of light, monochromators and detectors, Beer's law in chemical analysis, photometric accuracy- Ringbom Plot, derivative spectrophotometry (first and second order), optical rotatory dispersion and circular dichroism. Analysis of mixture-resolved and unresolved spectra, measurement of equilibrium constant: Scatchard Plot; Stoichiometry-method of continuous variation- the Jobs plot, Photometric titrations.

Unit 4 Fluorescence and Phosphorescence Spectrometry

- ☰ Introduction, physical and chemical principles, relaxation processes, Jalonski diagram, fluorescence, phosphorescence and structure, quantum yield, effect of structural rigidity, temperature, concentration and solvents, instrumentation, interferences (additive and multiplicative) and application for quantitative measurements.

REFERENCES

1. *“Quantitative Chemical Analysis”* by Daniel C. Harris, 7th Edition, W.H. Freeman and Company, New York, 2007.
2. *“Analytical Chemistry”* by Gary D. Christian, Purnendu K. (Sandy) Dasgupta and Kevin A. Schug, 7th Edition, John Wiley and Sons Inc. New Jersey, 2014.
3. *“Fundamental of Analytical Chemistry”* by Douglas A. Skoog, Donald M. West, F. James Holler, Stanley R. Crouch, 8rd Edition, Thomson, Brookes/Cole, 2004.
4. *“Modern Analytical Chemistry”* by David Harvey, McGraw Hill, New York, 2001.

M.SC. SEMESTER II PRACTICALS

CHE 411 PR INORGANIC CHEMISTRY (Minimum 9)

- ☰ Synthesis of metal complexes and salts;
1. Ferrous ammonium sulphate.
 2. Tris-acetylacetonato Manganese(III) chloride.
 3. Potassium trioxalato ferrate
 4. Potassium trioxalato Chromate
 5. Prussian blue
 6. Cis – trans- bis oxalate, diaquo chromate(III)
 7. Synthesis of penta amminechlorocobalt (III) chloride
 8. Preparation of tris -acetylacetonato iron(III)
 9. Preparation of manganese dioxide nano-particles
 10. Preparation of bis-chloro bis-triphenyl phosphine nickel (II)
 11. Synthesis of hexaammine cobalt(III) chloride
 12. Preparation of tetra-butylammoniumhexa molybdate (VI)

REFERENCES

1. *Practical Inorganic Chemistry: Preparations, reactions and instrumental methods*, G.Pass, ISBN: 978-94-017-2744-0, Springer.
2. *Experimental Inorganic/Physical chemistry*, M.A. Malati, 978-1-898563-47-1 Woodhead Publishing Ltd., Cambridge, UK.
3. *Some Experiments for M. Sc in Inorganic Chemistry*, Prof. J B Baruah, IIT, Gauahati.

M.SC. SEMESTER II PRACTICALS

CHE 411 PR ORGANIC CHEMISTRY (Minimum 9)

- ☞ One step preparation of organic compounds and study of general reaction, mechanism, mole ratio calculation, TLC, purification, IR and ¹HNMR (Theoretical)
- ☞ Distribution of Marks as per University exam: Principle and reaction mechanism (05 marks), Mole ratio and other calculation (05 marks), Crude and Crystal (10 marks), Purification, spectral data and M.P/B.P (05 marks), TLC (05 marks) and Viva (05 marks), Total 35 marks
- ☞ List of Preparations
 1. Sandmeyer reaction:
 - a. Preparation of *p*-chlorotoluene
 - b. Preparation of Iodo nitro benzene
 2. Beckmann rearrangement: Preparation benzanilide
 3. Cannizzaro reaction
 - a. Preparation of Benzoic acid
 - b. Preparation of Benzyl alcohol
 4. Coupling reaction: Preparation of benzapinacol
 5. Dyes
 - a. Preparation of Florescence
 - b. Preparation of Eosin
 6. Fischer Indole synthesis: 2-phenyl indole
 7. Polymerization: Preaparatoin of bakelite
 8. Reimer-Tiemann reaction: Preparation of β-hydroxynapthaldehyde
 9. Skraup synthesis: Preparation of quinoline
 10. Preparation of paracetamol
 11. Green reactions: Preparation of *p*-Bromo acetanilide from acetanilide

REFERENCES

1. *A text book of practical organic chemistry – A. I. Vogel*
2. *Practical organic Chemistry – Mann and Saunders*

M.SC. SEMESTER II PRACTICALS

CHE 412 PR PHYSICAL CHEMISTRY (Minimum 9)



Conductometry

1. To examine the validity of the Debye-Huckel-Onsagar (D.H.O) equation for strong electrolytes
2. To determine the hydrolysis constant of a salt of strong acid and weak base e.g. aniline hydrochloride.
3. To determine ion association constants (ion pair formation) of KCl in dioxane-water mixture.



Potentiometry

1. To find the stability constant of Ag-NH₃ complex.
2. To determine the heat of reaction, entropy change and equilibrium constant for the reaction between metallic Zinc and copper ions.



pH metry

1. To determine the solubility and dissociation constant of salicylic acid in ethanol-water mixture.
2. To determine the dissociation constant of a monobasic acid ClCH₂COOH and benzoic acid.



Chemical Kinetics and Adsorption

1. To study the reaction between acetone and iodine in presence of acids.
2. To study the autocatalytic reaction between KMnO₄ and H₂C₂O₄.
3. To determine the surface area of the given powdered catalyst sample by means of B.E.T. adsorption isotherm.
4. To study the adsorption of aqueous oxalic acid solution by activated charcoal and examine the validity of Freundlich and Langmuir's adsorption isotherms.

REFERENCES

1. *Practical physical chemistry –J.B.Yadav*
2. *Practicals in physical chemistry – P.S.Sindhu*
3. *Experimental physical chemistry – R.C.Das, B.Behera*
4. *Experiments in physical chemistry- P.H.Parsania, F. Karia*
5. *Experimental physical chemistry – V.D. Athawale, ParulMathur*
6. *Advanced physical chemistry experiments – Gurtu-and Gurtu*

M.SC. SEMESTER II PRACTICALS

CHE 412 PR ANALYTICAL CHEMISTRY (Minimum 10)

1. Determination of saponification value of oil.
2. Determination of iodine value of oil.
3. Determination of acid value of oil.
4. Determination of dissolved oxygen.
5. Determination of chemical oxygen demand.
6. Determination of iron in iron tablets.
7. Simultaneous estimation of chromium (III) and iron (III) by EDTA titration.
8. Simultaneous estimation of calcium (II) and zinc (II) by EDTA titration.
9. Simultaneous estimation of lead (II) and magnesium (II) by EDTA titration.
10. Separation of amino acids by TLC.
11. Separation of drugs by TLC.
12. Separation of dyes by TLC.
13. To determine Ca in Ginger sample.
14. Extraction of caffeine from dry tea leaves and its quantitative determination.

REFERENCES

1. *Analytical Chemistry: Practice, Second Edition, John H. Kennedy, Saunders College Publishing.*
2. *Vogel's Textbook of Quantitative Chemical Analysis, Fifth edition, Longman Scientific and Technical and John Wiley & Sons, Inc., New York.*

GUJARAT UNIVERSITY

MSc Analytical Chemistry Semester III and IV

Revised Syllabus

Design and Structure of Choice Based Credit System

(Effective from 2021-2022)

| MSc SEMESTER III | | | | | | |
|------------------|---|---|-------------------|-----------|------------------|------------|
| Course | | No. of hours per week (12 h for each unit and 48 h for each paper/course) | | | Total credits | Marks |
| Paper Code | Type | Lectures | Labs | Total | | |
| CHE(A) 501 | Core Paper | 4 | -- | 4 | 4 | 100 |
| CHE(A) 502 | Core Paper | 4 | -- | 4 | 4 | 100 |
| CHE(A) 503 | Core Paper | 4 | -- | 4 | 4 | 100 |
| CHE(EA) 504 | Elective Paper | 4 | -- | 4 | 4 | 100 |
| CHE(A) 505 PR | Lab Course-I | -- | 6 | 6 | 4 | 100 |
| CHE(A) 506 PR | Lab Course-II | -- | 6 | 6 | 4 | 100 |
| | Total | 16 | 12 | 28 | 24 | 600 |
| MSc SEMESTER IV | | | | | | |
| Course | | No. of hours per week (12 h for each unit and 48 h for each paper/course) | | | Total credits | Marks |
| Paper Code | Type | Lectures/ Discussion | DISS/PW and IT | Total | | |
| CHE(A) 507 | Core Paper | 4 | -- | 4 | 4 | 100 |
| CHE(A) 508 | Core Paper | 4 | -- | 4 | 4 | 100 |
| CHE(A) 509 | Industrial Training (IT) | -- | 5 | 5 | 4 | 100 |
| CHE(A) 510 | Dissertation (DISS)/ Project Work (PW) | -- | 15 | 15 | 12 | 300 |
| | Total | 08 | 20 | 28 | 24 | 600 |

For each paper 30 % weightage is given to internal assessment and 70 % for external assessment.

INDEX

| Subject | Page No. | |
|-------------------------------------|---|----|
| MSc SEMESTER III (Theory) | | |
| CHE(A) 501 | Separation Techniques and Bioanalytical Chemistry | 4 |
| CHE(A) 502 | Trends in Analytical Science | 7 |
| CHE(A) 503 | Electroanalytical Techniques | 10 |
| CHE(EA) 504 | EA-1. Industrial Analytical Chemistry | 13 |
| | EA-2. Thermal and Radiochemical Methods | 17 |
| | EA-3. Spectroscopic Techniques for Pharmaceutical and Biopharmaceutical Industries (Swayam Online Course) | 20 |
| MSc SEMESTER III (Practical) | | |
| CHE(A) 505 PR | Lab Course-I Experiments on Ion-exchange Chromatography, Thin layer Chromatography, Solvent extraction, Cloud Point extraction | 22 |
| CHE(A) 506 PR | Lab Course-II Experiments on Spectrophotometry, Fluorescence Spectroscopy, Flame Photometry, and Infrared Spectroscopy | 23 |
| <hr/> | | |
| MSc SEMESTER IV | | |
| CHE(A) 507 | Scientific Writing | 26 |
| CHE(A) 508 | Report Writing | 29 |
| CHE(A) 509 | Industrial Training | 31 |
| CHE(A) 510 | Dissertation/Project Work | 32 |

MSc SEMESTER III
ANALYTICAL CHEMISTRY

CHE(A) 501 SEPARATION TECHNIQUES AND BIOANALYTICAL CHEMISTRY

Learning Objective

- ☑ The main objective of this course is to familiarize students with the fundamental principles and working mechanism of separation tools/techniques used in analytical science such as, gas, liquid, and supercritical fluid chromatography, size exclusion, chiral, and affinity chromatography.
- ☑ Although modern chemical separation techniques are routinely practiced, the aim is to integrate all into one course.
- ☑ Although no hands-on training is provided, by completion of this course students are expected to gain theoretical method development skills in all separation techniques.
- ☑ The goal is to explain the chemical basis for stationary phase and mobile phase effects, to predict retention order given the relative dominance between stationary phase effects and mobile phase effects, to predict the effects of overloading, early and slow elution, baseline drift.
- ☑ Study in detail about quantitative bioanalysis, various stages of bioanalysis, bioanalytical method development and validation.

Learning Outcome

At the end of the course the students will be able to:

- ☑ Explain the principles of the most important liquid, supercritical fluid and gas chromatographic techniques.
- ☑ Evaluate strengths and limitations of the most important chromatographic separation and detection methods in relation to the properties of the sample.
- ☑ Interpret data from analytical separation methods.
- ☑ Choose and plan the use of suitable chromatographic technique for actual analytical problem solving with a reasonable degree of knowledge of potentially relevant methods.
- ☑ Be able to report and discuss chromatographic analyses in a scientifically sound, and understandable (intelligible) way.
- ☑ Account for the need of bioanalytical methods at projects within pharmacology, biopharmaceutics, pharmacokinetics, pharmacodynamics, metabolism, and toxicology
- ☑ Understand the basic principles of method construction and validation of bioanalytical methodology.

CHE(A) 501 Separation Techniques and Bioanalytical Chemistry

Unit 1 *Modern Liquid Chromatography*

- ◆ Principle, theory, and applications of ultra-performance liquid chromatography (UPLC), hydrophilic interaction liquid chromatography (HILIC), preparative high-performance liquid chromatography, flash chromatography, counter current chromatography, chiral chromatography, size/molecular exclusion/gel permeation chromatography and affinity chromatography, multidimensional liquid chromatography

Unit 2 *Gas Chromatography*

- ◆ Principle & theory, types of gas chromatography (GC) columns: packed and capillary columns, stationary phases-the key to different separations, temperature programming and carrier gas, types of sample injection, types of detectors: thermal conductivity, flame ionization, electron capture, flame photometric, flame thermionic and sulfur chemiluminescence detectors.
- ◆ Head space GC, pyrolysis GC, application in pharmaceutical, food, flavors, and fragrances analysis, multidimensional gas chromatography

Unit 3 *Supercritical Fluid Chromatography*

- ◆ Theory & historical development of supercritical fluid chromatography (SFC), carbon dioxide as the mobile phase, column selection, mobile phase additives & modifiers, effect of temperature & pressure, instrumentation for analytical and preparative SFC,
- ◆ Chiral & achiral SFC, applications in pharmaceuticals, food analysis and natural products

Unit 4 *Bioanalytical Chemistry*

- ◆ Quantitative bioanalytical method development: extraction from biological matrices, importance of internal standards, chromatography, and detection systems. Bioanalytical method validation parameters: sensitivity, selectivity, accuracy and precision, linearity (calibration curves), recovery, matrix effect, stability, dilution reliability, ruggedness
- ◆ Bioavailability and bioequivalence study, incurred sample reanalysis test for subject samples. US Food and Drug Administration (FDA) guidance for bioanalytical method validation, acceptance criterion

RECOMMENDED REFERENCES

- 1 *"Quantitative Chemical Analysis"*, Daniel C. Harris, 9th Edition, W.H. Freeman and Company, New York, 2015.
- 2 *"Analytical Chemistry"*, Gary D. Christian, 7th Edition, John Wiley and Sons Inc. New Jersey, 2004.
- 3 *"Fundamentals of Analytical Chemistry"*, Douglas A. Skoog, Donald M. West, F. James Holler, Stanley R. Crouch, 9th Edition, Cengage learning, 2016.
- 4 *"Principles of Instrumental Analysis"*, Douglas A. Skoog, F. James Holler, Stanley R. Crouch, 7th Edition, Cengage learning, 2017.
- 5 *"Modern HPLC for Practicing Scientists"*, Michael W. Dong, Wiley Interscience, 2006.
- 6 *"Ultra-high performance liquid chromatography and its applications"*, SzabolcsFekete, Julie Schappler, Serge Marc TancrèdeRudaz, Jean-Luc Veuthey, and Davy Guillarme, Edited by Quanyun A. Xu. New York: Wiley, 2013.
- 7 *"Chiral Separation Techniques: A Practical Approach"*, 2nd Edition, edited by Ganapathy Subramanian, Wiley-VCH, 2001.
- 8 *"Chiral Separations by Chromatography"*, Satinder Ahuja, American Chemical Society, 2000.
- 9 *"A Practical handbook of preparative HPLC"*, Donald Wellings, Elsevier, 2006.
- 10 *"Hydrophilic Interaction Chromatography"*, Bernard A. Olsen, Brian W. Pack, Hoboken: Wiley, 2013.
- 11 *"Perspectives on the future of multi-dimensional platforms"*, G. Groeneveld, B.W. Pirok, P.J. Schoenmakers, Faraday discussions, 218(2019)72-100.
- 12 *"Flash Chromatography System: A Practical Tool for Demonstrating the Influence of Column Characteristics on Chromatographic Resolution"*, A. Kasprowiak, F. Cazier-Dennin, P.E. Danjou, Journal of Chemical Education. 97 (2020) 1145-1150.
- 13 *"Countercurrent chromatography: People and applications"*, A. Berthod, M.J. Ruiz-Ángel, S. Carda-Broch, Journal of Chromatography A, 1216 (2009) 4206-4217.
- 14 *"Multidimensional Chromatography"*, L. Mondello, A.C. Lewis, K.D. Bartle, Chichester: Wiley, 2002(p. 109).
- 15 *"Gas Chromatography"*, Colin Poole, Elsevier Science, 2012.
- 16 *"Basic gas chromatography"*, Harold M. McNair, James M. Miller, Nicholas H. Snow, John Wiley & Sons, 2019.
- 17 *"Modern Supercritical Fluid Chromatography: Carbon Dioxide Containing Mobile Phases"* Larry M. Miller, J. David Pinkston, Larry T. Taylor, John Wiley & Sons, 2019.
- 18 *"Supercritical fluid chromatography"*, Colin F. Poole, ed., Elsevier, 2017.
- 19 *"Bioanalysis of Pharmaceuticals: Sample Preparation, Separation Techniques and Mass Spectrometry"*, Steen Honoré Hansen, Stig Pedersen-Bjergaard, eds., John Wiley & Sons, 2015.
- 20 *"Handbook of LC-MS bioanalysis: best practices, experimental protocols, and regulations"*, Wenkui Li, Jie Zhang, L.S. Francis, eds., John Wiley & Sons, 2013.
- 21 US Food and Drug Administration, *Guidance for Industry: Bioanalytical Method Validation*. US Department of Health and Human Services, Food and Drug Administration Centre for Drug Evaluation and Research and Centre for Veterinary Medicine, 2018.

CHE(A) 502 TRENDS IN ANALYTICAL SCIENCE

Learning Objective

- ☑ The overall goal of this course is to provide a resource that can be used to facilitate familiarity with basic concepts of the automation in the analytical measurements, significance of artificial intelligence, fundamentals of mass spectrometry and its related hyphenated techniques and green analytical chemistry.
- ☑ Automation in the measurements unveils the black-box and provides information/principles about process control, automatic & automated instruments to handle many samples and/or process, in the environmental and clinical laboratories.
- ☑ The ultimate aspiration of green analytical chemistry is the democratization of analytical chemistry.

Learning Outcome

Upon completion of the course, students will be able to:

- ☑ Understand types of automated instruments and devices commonly used and the principles behind their operation. Their application to process control and the techniques of flow injection analysis that allow most common analytical measurements to be performed automatically using microliter volumes of samples and reagents.
- ☑ Explain the mass spectrometric technique covering the fundamentals, terminology, data interpretation, hyphenated techniques, instrumentation, ion sources, mass analysers, detectors, and its applications.
- ☑ Acquire the skills to evaluate strengths and limitations of different hyphenated techniques with respect to sample properties and to specific analytical problems.
- ☑ Acquire the skills to find, choose and plan the use of suitable hyphenated techniques for actual advanced analytical problems based on a sound knowledge of the relevant method.
- ☑ Understand the 12 principles of green chemistry for analytical chemistry, through use of green solvents in the sample preparation and green chromatography.
- ☑ Design, develop and run all these techniques in a sustainable manner.
- ☑ Develop abilities to apply the knowledge and skills acquired to solve analytical problems associated with applications in real life.

CHE(A) 502 Trends in Analytical Science

Unit 1 *Automation in Measurement and Artificial Intelligence*

- ◆ Principles of automation, automatic and automated devices, Process control: off-line, at-line and on-line analysis. Continuous and discrete analyzers, feed-back mechanism
- ◆ Flow injection analysis (FIA), principles, dispersion coefficient, factors affecting peak height-sample volume, channel length, flow rate and channel geometry, Applications of FIA (chloride and phosphate determination), FIA acid-base titration, stopped flow measurements and gradient FIA, Artificial intelligence in analytical chemistry, Laboratory Information Management Systems (LIMS)

Unit 2 *Mass Spectrometry and HRMS*

- ◆ Principles of mass spectrometry, Ion sources: electron ionization and chemical ionization, electrospray ionization, atmospheric pressure chemical ionization (APCI), atmospheric pressure photo ionization (APPI) and atmospheric pressure secondary ion (APSI) mass spectrometry; matrix assisted laser desorption ionization (MALDI)
- ◆ Mass analyzers- quadrupole, ion-trap, time of flight (TOF), ion-cyclotron resonance and Fourier transform mass analyzers, High resolution mass spectrometry (HRMS), Tandem mass spectrometry, Applications

Unit 3 *Advanced Hyphenated Techniques*

- ◆ Principle, theory, instrumentation, working and applications of liquid chromatography-nuclear magnetic resonance-mass spectrometry (LC-NMR-MS), liquid chromatography-mass spectrometry/tandem mass spectrometry (LC-MS & LC-MS/MS), gas chromatography- mass spectrometry/tandem mass spectrometry (GC-MS & GC-MS/MS) and inductively coupled plasma-mass spectrometry (ICP-MS), Applications of hyphenated techniques

Unit 4 *Green Analytical Chemistry*

- ◆ Principles of Green Analytical Chemistry, Green Methodology in Analytical Sciences: Characteristics of green methods, Greening Sample Preparation: Strategies/techniques, New Sorbents, Green Solvents for Analytical Chemistry
- ◆ Green aspects for gas and liquid chromatography: State-of-the-art, Opportunities and Future Perspectives, Eco-scale metric approaches for evaluation of the greenness of analytical procedures

RECOMMENDED REFERENCES

- 1 *"Quantitative Chemical Analysis"*, Daniel C. Harris, 9th Edition, W.H. Freeman and Company, New York, 2015.
- 2 *"Analytical Chemistry"*, Gary D. Christian, 7th Edition, John Wiley and Sons Inc. New Jersey, 2004.
- 3 *"Fundamentals of Analytical Chemistry"*, Douglas A. Skoog, Donald M. West, F. James Holler, Stanley R. Crouch, 9th Edition, Cengage learning, 2016.
- 4 *"Principles of Instrumental Analysis"*, Douglas A. Skoog, F. James Holler, Stanley R. Crouch, 7th Edition, Cengage learning, 2017.
- 5 *"Taking the Leap between Analytical Chemistry and Artificial Intelligence: A Tutorial Review"*, L.B. Ayres, F.J. Gomez, J.R. Linton, M.F. Silva, C.D. Garcia, *Analytica Chimica Acta* 1161 (2021) 338403.
- 6 *"Laboratory Information Management Systems"*, Christine Paszko, Elizabeth Turner, 2nd Edition, CRC press, 2001.
- 7 *"Mass Spectrometry-Principles and Applications"*, Edmond de Hoffmann and Vincent Stroobant, John Wiley and Sons, 2007.
- 8 *"Mass Spectrometry: A Textbook"*, Jürgen H. Gross, Springer Science & Business Media, 2017.
- 9 *"Mass Spectrometry: An Applied Approach"*, 2nd Edition, Marek Smoluch, Giuseppe Grasso, Piotr Suder, Jerzy Silberring, eds., John Wiley & Sons, 2019.
- 10 *"High-Resolution Mass Spectrometry: An Emerging Analytical Method for Drug Testing"* In *Critical Issues in Alcohol and Drugs of Abuse Testing*, pp. 173-188, Michelle Wood, Academic Press, 2019.
- 11 *"LC/MS: A Practical User's Guide"*, Marvin C. McMaster, John Wiley and Sons, 2006.
- 12 *"On-line LC-NMR and related techniques"*, Klaus Albert (editor), John Wiley and Sons, 2002.
- 13 *"Recent progress in LC-NMR"*, T. Tokunaga, M. Okamoto, *Sumitomo Kagaku*, 2010(2): 40-48.
- 14 *"LC-NMR and other hyphenated NMR techniques"*, M.V. Silva Elipe, John Wiley & Sons, Inc, 2011.
- 15 *"Hyphenated techniques, applications of in mass spectrometry"*, W.M.A. Niessen, In *Elsevier Reference Module Chemical, Molecular Sciences and Engineering*, 2013.
- 16 *"GC/MS: A Practical User's Guide"*, Marvin C. McMaster, 2nd Edition, John Wiley and Sons, 2008.
- 17 *"Handbook of GC-MS: fundamentals and applications"*, Hans-Joachim Hübschmann, 3rd Edition, John Wiley & Sons, 2015.
- 18 *"Practical Guide to ICP-MS: A Tutorial for Beginners"*, Robert Thomas, 3rd Edition, CRC Press, 2013.
- 19 *"Handbook of Green Analytical Chemistry"*, Miguel de la Guardia, Salvador Garrigues, eds., West Sussex, UK: John Wiley & Sons, 2012.
- 20 *"Challenges in Green Analytical Chemistry"*, Salvador Garrigues, Miguel de la Guardia, RSC, 2020.
- 21 *"Green Analytical Chemistry: Past, Present and Perspectives"*, Justyna, Płotka-Wasyłka, Jacek Namieśnik, eds., Springer, 2019.

CHE(A) 503 ELECTROANALYTICAL TECHNIQUES

Learning Objective

- ☑ The fundamental goal of this course is to explain the importance of electroanalytical techniques for the analysis of chemicals and biochemicals and to facilitate in identification of the most appropriate electroanalytical technique for a specific analysis.
- ☑ To provide proficiency at evaluating the electrode reaction mechanism from data obtained using different electroanalytical techniques.
- ☑ To develop familiarity with electroanalytical techniques that are used for sensing of targets in research and industry.

Learning Outcome

Upon completion of the course, students will be able to:

- ☑ Identify the basic concept of electrochemical quantities for the basis of qualitative or quantitative measurement.
- ☑ Understand the basic concept of electrolysis for electrogravimetry and coulometric techniques under various conditions.
- ☑ Understand the instrumentation of electrogravimetry, coulometry technique.
- ☑ Recognize the application of electrogravimetry and coulometric technique.
- ☑ Learn problem solving for analytical tasks.
- ☑ Comprehend the advantages and disadvantages of various voltametric technique for selective and sensitive microanalysis.
- ☑ Understand the design of Ion-selective electrode, potentiometric and amperometric biosensors for detection of gases, biomolecules, and ions.
- ☑ Become familiar with biosensor techniques used in research and industry for analysis of biochemicals and chemicals.
- ☑ Learn electrochemical methods for sensing, including potentiometric sensors and biosensors, ion selective electrodes, amperometric sensors and conductometric sensors based chemiresistors.
- ☑ Be familiar with modern biosensing techniques such as field-effect transistors, biosensors based on chemiresistors and semiconducting oxide sensors.

Unit 1 *Electroanalytical Measurements*

- ◆ Introduction to potentiometry, galvanic measurements, potentiostatic measurements, voltage measurements with finite current, impedance measurements, electric double layer, electrocapillarity, current measurements, diffusion transport

Unit 2 *Electrodeposition and Coulometry*

- ◆ Fundamentals of electrolysis & current-voltage relationship,
- ◆ Electrogravimetry: principles, theory & types of electro gravimetric analysis at constant current, constant potential and at controlled potential, problems involved in electrogravimetry
- ◆ Coulometry: fundamentals, principle, theory & instrumentation, coulometric analysis at controlled potential coulometry, constant current coulometry, coulometric titration, applications of coulometric titration, comparison of constant current coulometry with conventional volumetric titration

Unit 3 *Voltammetry*

- ◆ Principle, theoretical consideration, basic experiment, instrumentation and applications of polarography, differential pulse polarography, square wave polarography, A.C. polarography, stripping analysis, cyclic voltammetry & amperometry titration

Unit 4 *Electrochemical and Biosensors*

- ◆ Potentiometric sensors and ion selective electrodes – concentration and activities, glass membrane type ISE, Gas sensing electrodes, Potentiometric biosensors linked with pH, NH₃, CO₂, Ag₂S and I₂
- ◆ Amperometric sensors- first generation, second generation and third generation, determination of glucose, lactate, cholesterol, phosphate, ethanol, starch, aspirin, and paracetamol using amperometric biosensor, amperometric gas sensors
- ◆ Conductometric sensors-chemiresistors, biosensors based on chemiresistors and semiconducting oxide sensors. Applications of Field-Effect Transistors sensors (Chemically Sensitive Field-Effect Transistors, Ion-Selective Field-Effect Transistors, FET-Based Biosensors)

RECOMMENDED REFERENCES

- 1 *"Quantitative Chemical Analysis"*, Daniel C. Harris, 9th Edition, W.H. Freeman and Company, New York, 2015.
- 2 *"Analytical Chemistry"*, Gary D. Christian, 7th Edition, John Wiley and Sons Inc. New Jersey, 2004.
- 3 *"Fundamentals of Analytical Chemistry"*, Douglas A. Skoog, Donald M. West, F. James Holler, Stanley R. Crouch, 9th Edition, Cengage learning, 2016.
- 4 *"Principles of Instrumental Analysis"*, Douglas A. Skoog, F. James Holler, Stanley R. Crouch, 7th Edition, Cengage learning, 2017.
- 5 *"Electroanalytical Chemistry-Principles, Best Practices, and Case Studies"*, Gary A. Mabbott, John Wiley & Sons, 2020.
- 6 *"Laboratory Techniques in Electroanalytical Chemistry"*, Peter T. Kissinger, William R. Heineman (Eds.), Marcel Dekker Inc., New York, 1996.
- 7 *"Electroanalytical Chemistry"*, Basil H. Vassos, Galen W. Ewing, John Wiley & Sons, New York, 1987.
- 8 *"Electrochemical Methods–Fundamentals and Applications"*, Allen J. Bard, Larry R. Faulkner, John Wiley & Sons, New York, 2001.
- 9 *"Treatise on analytical chemistry"*, E.B. Sandell. P. J. Elving, & I. M. Kolthoff (Eds.). Interscience, 1965.
- 10 *"Chemical Sensors and Biosensors"*, Brian R. Eggins, JohnWiley &Sons, NewYork, 2002.
- 11 *"Potentiometry and Ion Selective Electrodes"*, Alun Evans, ACOL by Wiley, 1987.
- 12 *"Analytical Chemistry"*, Dhruva Charan Dash, PHI Learning Private Limited, New Delhi.

M.Sc. SEMESTER III

CHE(EA) 504 INDUSTRIAL ANALYTICAL CHEMISTRY
(Elective Analytical-1)

Learning Objective

- ☑ The aim of this course is to provide students with a broad understanding of the principles of analytical chemistry and their application in the areas of environmental, food and food products, industrial materials, and agriculture. Depending on their project, the students will have the opportunity to apply analytical chemical methods in any one of the aforementioned areas.
- ☑ To aware students critically about their roles and identities as a consumers and environmental actors in a complex, interconnected world.
- ☑ To provide knowledge on the key food safety, their methods of detection and the key food quality properties.
- ☑ To provide the knowledge of the proper procedures and regulations for safe handling and use of chemicals.

Learning Outcome

Upon completion of the course, students will be able to:

- ☑ Describe and compare a range of analytical chemistry methods and explain the underlying theoretical principles.
- ☑ Explain the broad role of analysts in quality control and assessment of experimental measurements from various application contexts especially environmental analysis, food analysis, analysis of industrial materials like alloys, cement, paints, pigments, & petrochemical products, and analysis of fertilizers, soaps & detergents.
- ☑ Employ a variety of analytical methods to prepare, separate and characterise samples from various matrices.
- ☑ As part of a team or individually, conduct, analyse and interpret results of a chemical analysis and effectively communicate these in written reports and other formats.
- ☑ Learn the ability to work safely and competently in an analytical laboratory setting.

Unit 1 *Environmental Analysis*

- ♦ Analysis of Air: Sampling and examination of airborne solids, Direct instrumental methods for gaseous pollutants, Sampling of gases and the atmosphere, Gas chromatography, some chemical methods for determining trace gases
- ♦ Analysis of Water: The analysis of water, Selected analytical methods for water quality control, pH measurement – the glass electrode, Conductivity, Dissolved oxygen (DO), Biochemical oxygen demand (BOD), Chemical oxygen demand (COD), Methods for the determination of inorganic nitrogen, Determination of phosphate, Automation of colorimetric procedures, titrimetric determination of chloride, Ion-selective electrodes, Ion chromatography, The determination of heavy metals, The importance of chemical species – speciation, Trace organics in water – total organic carbon (TOC), Determination of some individual compounds or groups of compounds in polluted water, Gas chromatography/mass spectrometry (GC/MS)
- ♦ Soil Analysis: Sampling of soil, pH of Soil, moisture determination by Karl Fischer titration methods, Determination of total nitrogen, ammonia and nitrates, Estimation of available Nitrogen (Kjeldahl's Method), determination of total phosphates as P_2O_5 , Soil analysis for micronutrients

Unit 2 *Food Analysis*

- ♦ Analysis of food: Introduction to food analysis, regulations and international standards related to food analysis, nutritional labeling, sampling, and sample preparation
- ♦ Compositional analysis of foods: moisture, proteins, fat, fiber, ash, vitamins and minerals, Adulteration of fats and oils, milk, and milk products
- ♦ Analysis of food products for flavoring agents, colour and various contaminants
- ♦ Analysis of Oils & Fats: Theory, Melting point of fats, Chemical Characteristics: saponification value, iodine value, acid value, thiocyanogen value, ketone, or perfume rancidity. Analysis of fatty acid composition in oils by GLC, Oxidation levels of fats by TLC

Unit 3 *Analysis of Industrial Materials*

- ♦ Analysis of Ferroalloys: Analysis of steel - Molybdenum, Phosphorous. Analysis of Ferromanganese, Ferrovandium. Analysis of non- Ferrous alloys: Analysis of Tin, Zinc and Copper in Brass, Bronze. Analysis of Tin and lead in Solder
- ♦ Analysis of Cement: Composition of Portland cement, estimation of Aluminium

oxide and Ferrous oxide. Determination of Alumina in Cement by Polarography

- ♦ Paints and Pigments: Types of paints and pigments, determination of volatile and non-volatile components, Flash point (significance and method of determination), separation and analysis of pigments. Analysis of TiO₂ in Titanium dioxide pigments by XRD. Determination of Zn, Pb in Paint pigments by Polarographic method. Analysis of polyesters, acrylics by Gel permeation chromatography
- ♦ Petrochemical Products: Classification of Petrochemical products: crude oils, fuels, and calorific values, fractional distillation process and fractions, properties of fuel, composition of fuel, flashpoint, fire point, corrosion test, carbon residue

Unit 4 Analysis of Pesticides, Fertilizers, Soaps, and Detergents

- ♦ Pesticides: Introduction, Classification and properties of pesticides based on mode of action, targeted pest species and chemical composition, Physical and chemical properties of pesticides, Analysis of different pesticides by classical and instrumental methods
- ♦ Fertilizers: Types of fertilizers and analysis of different elements like nitrogen, phosphates, calcium, sodium, potassium, and ammonia
- ♦ Soaps and detergents: Classification of soaps and detergents with suitable examples, the chemistry of soaps and detergents, properties and characterization of soaps and detergents: Alkali and total fatty matter, active ingredients and oxygen releasing capacity

RECOMMENDED REFERENCES

- 1 *"Analytical Chemistry"*, Gary D. Christian, 7th Edition, John Wiley and Sons Inc. New Jersey, 2004.
- 2 *"Principles of Instrumental Analysis"*, Douglas A. Skoog, F. James Holler, Stanley R. Crouch, 7th Edition, Cengage learning, 2017.
- 3 *"Environmental Pollution Analysis"*, S. M. Khopkar, New Age International publication, 2011.
- 4 Guidelines for Drinking-Water Quality: 4th Edition Incorporating the First Addendum. Geneva: World Health Organization; 2017. Available from: <https://www.ncbi.nlm.nih.gov/books/NBK442376/>
- 5 *"Soil pollution"*, S.G. Misra, Dinesh Mani, APH Publishing Corporation, 2009.
- 6 *"Standard Method of Chemical Analysis"*, F.J. Welcher, 6th Edition, Volume 1,2 & 3, Part two, Van Nostrand Reinhold Company.
- 7 *"Principles of Environmental Chemistry"*, E. James Girard, Jones and Bartlett Publishers, 3rd Edition, 2013.
- 8 *"Food Analysis"*, S. Suzanne Nielsen, 5th Edition, Springer 2017.
- 9 *"Food Analysis Laboratory Manual"*, S. Suzanne Nielsen, 3rd Edition, Springer 2017.
- 10 *"Advanced Dairy Chemistry"*, P.L. McSweeney, P.F. Fox (Eds.), Boston, MA, USA: Springer; 2003.

- 11 *"Food Analysis: Theory and Practice"*, Y. Pomeranz, Ed., Springer Science & Business Media, 2013.
- 12 *"Food contaminants: Sources and surveillance"*, C. Creaser, R. Purchase (Eds.), Elsevier, 1991.
- 13 FSSAI (Food Safety and Standards Authority of India) Manuals of Methods of Analysis of Foods (Oils and Fats, Milk and Milk Products, Food Additives), Ministry of Health and Family Welfare, Government of India.
- 14 *"The Chemical Analysis of Foods and Food Products"*, 2nd Edition, M.B. Jacobs, 1951.
- 15 *"Analytical Agricultural Chemistry"*, 6th Edition, S.L. Chopra, J.S Kanwar, New Delhi, Kalyani publication, 2014.
- 16 *"Methods in Agricultural Chemical Analysis"*, N.T. Fainthfull, CABI Publishing, 2002.
- 17 *"Analysis of Pesticides in Food and Environmental Samples"*, José L. Tadeo (ed.), 2nd Edition, CRC Press, 2019.

**CHE(EA) 504 THERMAL AND RADIOCHEMICAL METHODS
(Elective Analytical-2)**

Learning Objective

- ☑ The aim of this course is to provide fundamental and practical aspects of thermal analysis and radiochemical methods.
- ☑ To give an overview of various thermal methods (TGA, DTA, DSC, TMA and EGA) and show how they can be used to measure different kinds of thermal events. Further, combined methods of thermal analysis and the interpretation of experimental results will be taught.
- ☑ The intent to incorporate radiochemical methods in this course is to give a thorough introduction to radioactivity as well as central concepts in radiochemistry. Radiochemical principles are seen in conjunction with chemical concepts and other fields where radiochemical principles can be utilized, such as the industry, the environment and medicine.
- ☑ The course shall relay knowledge about the role of radioactivity, both as a tool and its own scientific discipline. Applications where radiochemistry plays an integral part will be specifically treated.

Learning Outcome

After completing this course, students will be able to:

Thermal Methods

- ☑ Explain the basic principle and instrumentation of various thermal methods.
- ☑ Choose the experimental conditions for specific measurements.
- ☑ Identify the properties present in the various thermal methods.
- ☑ Consider factors, which affect thermal measurements.
- ☑ List the uses of each of the different thermal methods.
- ☑ Interprets related thermograms.

Radiochemical Methods

- ☑ Define radioactive decay processes and nuclear radiation.
- ☑ Know the principles of utilizing radioactivity applied to chemistry, chemical processes, and adjacent fields where chemistry is an integral part.
- ☑ Know the principles of radiation hygiene and the interaction of radiation and matter.
- ☑ Perform calculations in radiochemistry and utilize these in applied radiochemical sciences.
- ☑ Assess radiation and radiation exposure from a radiation protection point of view.

CHE(EA) 504 Thermal and Radiochemical Methods

Unit 1 *Thermogravimetry and Derivative Thermogravimetry*

- ◆ Introduction to Thermogravimetric Analysis (TGA), basic principles of TGA, derivative TGA, modern TGA instrumentation, mechanisms of weight change in TGA, classification of TGA curves, simultaneous TGA techniques, applications of TGA

Unit 2 *Differential Thermal Analysis and Differential Scanning Calorimetry*

- ◆ Introduction to Differential Thermal Analysis (DTA), basic principles of DTA, modern DTA instrumentation, factors affecting DTA curve, applications of DTA
- ◆ Introduction to Differential Scanning Calorimetry (DSC), basic principles of DSC, modern DSC instrumentation: power compensated, heat flux, modulated DSC instruments, DSC sensors, applications of DSC

Unit 3 *Thermomechanical and Evolved Gas Analysis*

- ◆ Introduction of Thermomechanical Analysis (TMA), basic principles of TMA, modern TMA instrumentation, types and selection of probes, applications of TMA
- ◆ Basic Principles of Evolved Gas Analysis (EGA), instrumentation, evolved Gas detection, mass spectrometry, Fourier transform infrared (FTIR) spectroscopy, gas chromatography, coupling the TGA to gas analyzer, applications of EGA

Unit 4 *Radiochemical Methods*

- ◆ Radioactive Nuclides: Radioactive decay products, decay processes, radioactive decay rates, counting statistics
- ◆ Instrumentation: Measurement of alpha particles, beta particles and gamma radiation
- ◆ Neutron activation methods: Neutrons and neutron sources, interactions of neutrons with matter, theory of activation methods, experimental considerations in activation methods, applications of neutron activation
- ◆ Isotope dilution methods: Principles and application of the isotope dilution procedure
- ◆ Radiometric titrations: Principle, types, and application of Radiometric titrations

RECOMMENDED REFERENCES

- 1 *"Principles of Instrumental Analysis"*, Douglas A. Skoog, F. James Holler, Stanley R. Crouch, 7th Edition, Cengage learning, 2017.
- 2 *"Principles of Thermal Analysis and Calorimetry"*, Peter Haines, Royal society of chemistry, 2001.
- 3 *"Introduction to Thermal Analysis: Techniques and Applications"*, Michael Ewart Brown, Vol. 1. Springer Science & Business Media, 2001.
- 4 *"Principles and Applications of Thermal Analysis"*, Paul Gabbott, ed, John Wiley & Sons, 2008.
- 5 *"Thermal Analysis in Practice: Fundamental Aspects"*, Matthias Wagner, ed, Carl Hanser Verlag GmbH Co KG, 2017.
- 6 *"Handbook of thermal analysis and Calorimetry: Recent Advances, techniques and applications"*, Sergey Vyazovkin, Koga Nobuyoshi, Christoph Schick. Elsevier Science, 2018.
- 7 *"Nuclear and Radiochemistry"*, 2nd Edition, K. H. Lieser, Weinheim, Germany: Wiley-VCH, 2001.
- 8 *"Handbook of Radioactivity Analysis"*, M. F. L'Annunziata, ed., San Diego: Academic Press, 1998.
- 9 *"Chemical Analysis by Nuclear Methods"*, Z. B. Alfassi, ed., Chichester, UK: Wiley, 1994.
- 10 *"Radiochemistry and Nuclear Methods of Analysis"*, W. D. Ehmann and D. E. Vance, New York: Wiley, 1991.
- 11 *"Radiochemistry and Nuclear Chemistry"*, G. R. Choppin, J. Rydberg, J. O. Liljenzin, C. Ekberg, 4th Edition, Oxford, UK: Academic Press, 2013
- 12 *"Nuclear and Radiochemistry: Fundamentals and Applications"*, Jens-Volker Kratz, Karl Heinrich Lieser, 3rd Edition, Wiley-VCH, 2013.
- 13 *"Nuclear and radiochemistry"*, József Kónya, Noémi M. Nagy, 2nd Edition, Elsevier, 2018.
- 14 *"Handbook of Nuclear Chemistry"*: Vol. 1: Basics of Nuclear Science; Vol. 2: Elements and Isotopes: Formation, Transformation, Distribution; Vol. 3: Chemical Applications of Nuclear Reactions and Radiation; Vol. 4: Radiochemistry and Radiopharmaceutical Chemistry in Life Sciences; Vol. 5: Instrumentation, Separation Techniques, Environmental Issues; Vol. 6: Nuclear Energy Production and Safety Issues, Attila Vértes, Sándor Nagy, Zoltán Klencsár, Rezso György Lovas, Frank Rösch, eds., 2nd Edition, Springer Science & Business Media, 2010.

M.Sc. SEMESTER III
CHE(EA) 504

**SPECTROSCOPIC TECHNIQUES FOR PHARMACEUTICAL AND
BIOPHARMACEUTICAL INDUSTRIES**
(SWAYAM ONLINE COURSE)
(Elective Analytical-3)

https://onlinecourses.nptel.ac.in/noc21_cy43/preview

About the Course

- ☑ A variety of spectroscopic techniques will be discussed along with their application in chemical, pharmaceutical and Bio-pharmaceutical Industries.
- ☑ Category: **1. Chemistry**
- ☑ Course Credit: **3**
- ☑ Course Duration: **12 weeks**

Course Certificate

- ☑ Average assignment score = 25% of average of best 8 assignments out of the total 12 assignments given in the course.
- ☑ Exam score = 75% of the proctored certification exam score out of 100
- ☑ Final score = Average assignment score + Exam score
- ☑ ELIGIBILITY CRITERIA FOR A CERTIFICATE: ONLY IF AVERAGE ASSIGNMENT SCORE $\geq 10/25$ AND EXAM SCORE $\geq 30/75$. If one of the 2 criteria is not met, the certificate will not be provided even if the Final score $\geq 40/100$.

CHE(EA) 504 Spectroscopic Techniques for Pharmaceutical and Biopharmaceutical Industries

(Swayam Online Course)

Course layout

- ♦ **Week 1:** Summary of spectroscopic techniques, electromagnetic radiation and its interaction with matter
- ♦ **Week 2:** Schrodinger Equation, Postulates of quantum mechanics, resolution, signal to noise ratio.
- ♦ **Week 3:** Rotational/ Rotational Raman and their application and Vibrational Spectroscopy
- ♦ **Week 4:** Application of Vibrational spectroscopy, Vibrational, Rotational-Vibration, Raman spectroscopy/Rotational-Raman/Vibrational-Raman
- ♦ **Week 5:** Atomic Spectroscopy
- ♦ **Week 6:** Flame photometry, AAS, ICP and its application, Molecular spectroscopy
- ♦ **Week 7:** Electronic spectroscopy, UV-Vis Spectroscopy and its application
- ♦ **Week 8:** Application of UV-Visible spectroscopy, Fluorescence spectroscopy
- ♦ **Week 9:** Fluorescence spectroscopy, Time resolved Spectroscopy
- ♦ **Week 10:** Microscopy
- ♦ **Week 11:** Mass spectroscopy, NMR spectroscopy
- ♦ **Week 12:** Application of FTIR, NMR and Mass in Pharmaceutical and Biopharmaceutical Industry

RECOMMENDED REFERENCES

- 1 *"Engineering Chemistry"*, P.B. Joshi and Shashank Deep, Oxford University Press, 2019.
- 2 *"Modern Spectroscopy"*, J. M. Hollas, John Wiley & Sons, 2004.
- 3 *"Absolutely Small: How Quantum Theory Explains our Everyday World"*, Michael D. Fayer, Amacom, 2010.
- 4 *"Fundamentals of Molecular Spectroscopy"*, C. N. Banwell & E.M. McCash, 1972.
- 5 *"Organic Spectroscopy"*, William Kemp, Springer, 1975.
- 6 *"Understanding light microscopy: Jeremy Sanderson"*, John Wiley & Sons, 2019.
- 7 *"Understanding NMR spectroscopy"*, James Keeler, John Wiley & Sons, 2005.
- 8 *"Principle of Fluorescence Spectroscopy"*, J.R. Lakowicz (Ed.), Springer, 2013.

CHE(A) 505 PR

Experiments: Ion-exchange Chromatography, Thin layer Chromatography, Solvent extraction, Cloud Point extraction (Minimum: 12)

- 1 Determination of ion-exchange capacity of cation and anion exchangers.
- 2 Ion-exchange separation and determination of halides (chloride and bromide) on anion exchange column.
- 3 Ion-exchange separation and determination of zinc and magnesium on anion exchange column.
- 4 Ion-exchange separation and determination of cadmium and zinc on an anion exchanger column.
- 5 Separation and determination of multiple analytes (three or more drugs) using TLC and HPTLC.
- 6 Extraction and determination of food colours (tartrazine, erythrosine, sunset yellow) from commercially available food samples using cloud point extraction (confectionary items).
- 7 Determination of nitrogen content of fertilizers (Kjeldahl's method).
- 8 Determination of alkali content & total fatty matter in cleansing agents (Soaps and detergents)
- 9 Estimation of drugs by non-aqueous titration: pyridoxine hydrochloride or sulphamethoxazole.
- 10 Determination of glucose from glucon D by titration with Fehling solution.
- 11 Determination of silica by molybdenum blue method
- 12 Estimation of caffeine in tea
- 13 Determination of calcium in milk powder using EDTA.
- 14 Determination of strength of commercial phosphoric acid by pH titration
- 15 Determination of ammonia in household cleaners by conductometric titrations.
- 16 Isolation/extraction of casein and lactose from milk and separation by TLC
- 17 Determination of iron in mustard sugar, phosphorus in peas, ascorbic acid in tomato, benzoic acid in food products
- 18 Analysis of the composition of a mixture of nitroanilines by thin-layer chromatography and ultraviolet-visible spectrometry

RECOMMENDED REFERENCES

- 1 "Vogel's Textbook of Quantitative Chemical Analysis", I. Vogel, 5th Edition, Revised by G.H. Jeffery, J. Bassett, J. Mendham, R.C. Denny, Longman House, Burnt Mill, Harlow. Essex CM20 2JE, England, 1989.
- 2 "Vogel's Textbook of Quantitative Chemical Analysis", I. Vogel, 6th Edition, Revised by J. Mendham, R.C. Denny, J.D. Barnes, M.J.K. Thomas, Pearson Education, India, 2000.
- 3 "Analytical Chemistry", Gary D. Christian, 7th Edition, John Wiley and Sons Inc. New Jersey, 2004.
- 4 "Quantitative Chemical Analysis", Daniel C. Harris, 9th Edition, W.H. Freeman and Company, New York, 2015.

M.Sc. SEMESTER III

CHE(A) 506 PR ANALYTICAL CHEMISTRY PRACTICALS

Lab Course-II

CHE(A) 506 PR

Experiments: *Experiments on Spectrophotometry, Fluorescence Spectroscopy, Flame Photometry, and Infrared Spectroscopy (Minimum: 12)*

- 1 Spectrophotometric determination of binary mixture (KMnO_4 and $\text{K}_2\text{Cr}_2\text{O}_7$) when their spectra do not overlap.
- 2 Spectrophotometric determination of binary mixture (Titanium and Vanadium) when their spectra overlap.
- 3 Spectrophotometric determination of ionization constant of an indicator (bromothymol blue).
- 4 Spectrophotometric determination of pKa of methyl red indicator
- 5 Determination of stoichiometry of Fe(II)-1,10-phenanthroline complex by Job's method of continuous variation.
- 6 Simultaneous spectrophotometry (zero order, first and second derivative) determination of drugs.
- 7 Spectrophotometric determination of nitrate nitrogen in water.
- 8 Spectrophotometric determination of lead in leaves using solvent extraction.
- 9 Ultraviolet spectrophotometric determination of aspirin, phenacetin and caffeine in APC tablet using solvent extraction.
- 10 Simultaneous determination of arsenic (III) and antimony (III) in a mixture using bromate/bromide solution by spectrophotometry.

- 11 Determination of stability constants/formation constants of metal-complexes by spectrophotometry (Scatchard Plot).
- 12 Quantitative analysis of charge transfer complexes of iodine with drugs by spectrophotometry (linearity, accuracy, and precision).
- 13 Determination of Na and K in commercial samples by flame photometry.
- 14 Quantitative analysis of riboflavin (Vitamin B₂) in energy drinks by fluorescence spectroscopy.
- 15 IR Spectroscopy for detection of primary, secondary, and tertiary amines
- 16 IR Spectroscopy for detection of carbonyl functionality in acid, amide, aldehyde, and ketone.
- 17 Analysis of pesticides in environmental samples by Gas Chromatography-Mass Spectrometer
- 18 Pre-concentration of copper, cobalt, nickel, and zinc from brine/sea water on Chelex-100 resin and their simultaneous determination using atomic absorption spectrophotometry.

RECOMMENDED REFERENCES

- 1 *"Vogel's Textbook of Quantitative Chemical Analysis"*, I. Vogel, 5th Edition, Revised by G.H. Jeffery, J. Bassett, J. Mendham, R.C. Denny, Longman House, Burnt Mill, Harlow. Essex CM20 2JE, England, 1989.
- 2 *"Vogel's Textbook of Quantitative Chemical Analysis"*, I. Vogel, 6th Edition, Revised by J. Mendham, R.C. Denny, J.D. Barnes, M.J.K. Thomas, Pearson Education, India, 2000.
- 3 *"Analytical Chemistry"*, Gary D. Christian, 7th Edition, John Wiley and Sons Inc. New Jersey, 2004.
- 4 *"Quantitative Chemical Analysis"*, Daniel C. Harris, 9th Edition, W.H. Freeman and Company, New York, 2015.

MSc SEMESTER IV
ANALYTICAL CHEMISTRY

M.Sc. SEMESTER IV

CHE(A) 507 SCIENTIFIC WRITING

Learning Objective

- ☑ The purpose of scientific writing is to help students analyse and clarify their thinking about a particular topic, synthesize their ideas, and communicate them with others. The different options offered to students are specific in nature and serve a distinct purpose.
- ☑ To generate scientific temper and understanding among students to articulate their thinking as they engage in the scientific practices. Scientific writing will serve as an effective means to increase student engagement in learning as well as to improve their academic success.
- ☑ The students are expected to design, execute, and publish a study through this writing-intensive course.

Learning Outcome

Upon completion of the course, the students

- ☑ Will understand the importance of literature survey in research.
- ☑ Will learn to carry out investigations, analysing and interpreting data, and constructing explanations.
- ☑ Shall start to become better readers, thinkers, and learners in their discipline by processing their ideas through writing.
- ☑ Benefit in preparing the day-in and day-out communicative tasks that they face on the job.
- ☑ Will build new scientific understanding as it provides students the opportunity to articulate their thinking as they engage in the science practices during an investigation.

CHE(A) 507 Scientific Writing

- ◆ Writing of Research Article/Review Article/Commentary Article/Case Study/Monograph/Book Chapter/Book Review/Research Proposal or any other scientific article type.
- ◆ The student can select any one scientific writing type or research proposal and submit a copy (hard and soft) of the same for internal and external evaluation.
- ◆ Evaluation will be centered around on novelty, relevance, significance, and impact.
- ◆ Additional weightage will be given for submission/publishing of any article type in any journal (University journal or a journal that is indexed in the UGC CARE list/Web of Science/ SCOPUS/SCI/SCIE etc.) or a research proposal.

Guidelines for Scientific Writing

Research Article

Presents a full report with new results on a specific topic. Complete experimental details with proper justification. Generally not limited in length, with figures, tables, and references. Format...Title, Authors, Abstract, introduction, experimental, results, discussion, conclusion, acknowledgment, references

Review Articles/Commentary Article

Gives an overview of research in a particular field. It can be on one's own research or any other topic of general and current interest. Organized differently from communications or research articles as it does not have primary experimental data. Data of existing literature can be presented in a tabular format, graphs, diagrams, figures, charts etc. Should be referenced as thoroughly as possible. Format...Title, Authors, Abstract, introduction, discussion, conclusion, acknowledgment, references

Case Study

This study represents person, group, or situation that has been studied over time. Format depends upon the type of study.

Monograph

Title, Author, Introduction: Reason to select a topic; History, timeline, and Scientific/social significance; Benefits to the scientific community, teaching, and research, Development: Exposition of ideas into paragraphs or chapters. "Quote that author endorse these ideas." Conclusion: Status and future perspectives, References: Should be referenced as thoroughly as possible

Book Chapter

Title, Authors, Abstract, Introduction/Background on the topic, Discussion (with subdivisions): Text with tables, figures, charts etc., Summary/Conclusion: Status and future perspectives, References

Book Review

A book review is a thorough description, critical analysis, and/or evaluation of the quality, meaning, and significance of a book, often written in relation to prior research on the topic.

Scope/Purpose/Content, Note the Method/Methodology of writing, Critically Evaluate the Contents, Examine the Front Matter and Back Matter, Summarize and Comment.

Research Proposal

Title, Research Problem/Problem Statement, Rational/Purpose of the Study
Review of the Literature, Proposed Research Framework, Research Questions/Proposed Hypothesis, Significance, Proposed Methods and Procedures, Deliverables/Expected Outcomes, Execution timelines, year wise breakup, financial aspects, References

RECOMMENDED REFERENCES

- 1 *"A Manual for Writers of Research Papers, Theses, and Dissertations"*, Kate Turabian, University of Chicago Press, 8th Edition, 2013.
- 2 *"Concise Guide to Writing Research Papers (Perfect Phrases Series)"*, Carol Ellison, McGraw-Hill Education; 1st Edition, 2010.

M.Sc. SEMESTER IV

CHE(A) 508 REPORT WRITING

Learning Objective

- ☑ The main purpose of writing a conference/seminar report is to provide an opportunity to the students to participate, present new findings through oral/poster presentations, interact with researchers/experts in different areas of Chemistry, and develop skill to summarise an event.
- ☑ It can serve as a platform for sharing experiences.

Learning Outcome

Upon completion of the course, students will be able to:

- ☑ Sharpen writing skills when it comes to details with good accuracy.
- ☑ Learn the best practices, methods and resources in research, presentation of own ideas.
- ☑ Learn from the experts.
- ☑ Expand network with researchers working in their areas of interest, for fulfilling career goals.
- ☑ Keep with the current trends.
- ☑ Build confidence as presenting at a conference is the perfect opportunity.

CHE(A) 508 Report Writing

- ◆ Report Writing for Participation and/or presentation (Poster/Oral/Invited talk as applicable) in University/State level/National/International Seminar/Conference/Webinar/ Symposium/Workshop/Hands-on training /Software learning of at least 2 days. In case of one day seminar/ webinar/ conference/workshop, it is mandatory to participate in two such events.
- ◆ Evaluation will be based on detailed technical report prepared on the conference/seminar/workshop participated and for Poster/Oral presentation, as applicable.
- ◆ Additional weightage will be given for Oral or Poster Presentation.

Guidelines for Report Writing

It aims to summarise the most important talks/research presented. It is not usually feasible to attempt comprehensive coverage of the conference. More focus should be on those presentations that are most topical, interesting, or thought-provoking.

Points to consider when writing the report:

- Name of Institute/Department/University that organized the conference
- Title and theme of the conference
- Information regarding number of attendees, where and when it was held (date), name of the convener, organizing secretary etc.
- Include a copy of the brochure
- A brief about the Inaugural Session
- Details of all the technical sessions
- List of main speakers, their position/designation, topic, expertise, and their institutional affiliation
- Highlight research paper(s) or work with major significance and impact
- A brief about the Concluding/Valedictory Session
- Embed the text with photographs wherever possible
- The outcome/summary: Your learning

RECOMMENDED REFERENCES

- 1 *“Writing for Conferences: A Handbook for Graduate Students and Faculty”*, Leo Mallette, Clare Berger, Greenwood; Illustrated Edition, 2011.
- 2 *“The Creative Writing Handbook”*, John Singleton (Editor), Mary Luckhurst (Editor), Red Globe Press; 2nd Edition, 1999.

M.Sc. SEMESTER IV
CHE(A) 509 INDUSTRIAL TRAINING

CHE(A) 509 Industrial Training

Guidelines for Industrial Training

- 1 Each student must undergo 3 weeks industrial training under the supervision of a faculty from the concerned department.
- 2 The industry may be in Ahmedabad, Gujarat or anywhere in India.
- 3 The training may be obtained at any R&D, QA, QC, Production or any other relevant department on different instrumental techniques or other laboratory equipments.
- 4 The students must submit a report on the training obtained from the industry which may include (a) introduction about the industry (b) various activities of the industry (c) the process which are used in the industry (d) the products of the industry and (e) summary and conclusion.
- 5 The report submitted by each student would be assessed by the branch in-charge and the supervising teacher.
- 6 The student must discuss/present the details of the training through a power point presentation

CHE(A) 510 Dissertation/Project Work

Guidelines for Dissertation/Project Work

- 1 Each student must carry out a project under the supervision of a faculty from the concerned department.
- 2 The project can be carried out either in the department or in any other industry, institute or organizations located in Ahmedabad, Gujarat or anywhere in India.
- 3 The topics of the dissertation can be selected from any of the four branches of chemistry i.e., Organic, Inorganic, Physical or Analytical. The topic can be related to (a)synthesis, purification, characterization, application of organic compounds or (b)metal complexes preparation and applications or (c)physical studies of various systems (d) method development and validation (e) green chemistry (f) nanomaterials preparation and applications (g) functionalized supramolecules (h) electro analytical methods (i) environmental analysis and decontamination or any other related to the subject.
- 4 Each student must submit a dissertation on the topic of their study comprising of (a) an introduction on the topic along with literature survey and justification for the selection of the topic (b) materials and methods (c) methodology (d) results and discussion and (e) summary and conclusion along with the references.
- 5 Each student must give monthly report and a midterm presentation of their work at the department.
- 6 The student must discuss/present the details of dissertation through a power point presentation.
- 7 Dissertation would be examined by the supervising teacher and external examiner.

GUJARAT UNIVERSITY
MSc Inorganic Chemistry Semester III and IV
Revised Syllabus
Design and Structure of Choice Based Credit System
(Effective from 2021-2022)

| MSc Semester III | | | | | | |
|-------------------------|---------------------------------------|--|-------------------|-------|---------------|-------|
| Course | | No. of hours per week (12 h for each unit and 48 h for each paper/course) | | | Total credits | Marks |
| Paper Code | Type | Lectures | Labs | Total | | |
| CHE (I) 501 | Core Paper | 4 | -- | 4 | 4 | 100 |
| CHE (I) 502 | Core Paper | 4 | -- | 4 | 4 | 100 |
| CHE (I) 503 | Core Paper | 4 | -- | 4 | 4 | 100 |
| CHE (EI) 504 | Elective Paper | 4 | -- | 4 | 4 | 100 |
| CHE (I) 505 PR | Lab Course 1 | -- | 6 | 6 | 4 | 100 |
| CHE (I) 506 PR | Lab Course 2 | -- | 6 | 6 | 4 | 100 |
| | Total | 16 | 12 | 28 | 24 | 600 |
| MSc Semester IV | | | | | | |
| Course | | No. of hours per week (12 h for each unit and 48 h for each paper/course) | | | Total credits | Marks |
| Paper Code | Type | Lectures/ Discussion | DISS/PW and IT | Total | | |
| CHE (I) 507 | Core Paper (Scientific Writing) | 4 | -- | 4 | 4 | 100 |
| CHE (I) 508 | Core Paper (Report Writing) | 4 | -- | 4 | 4 | 100 |
| CHE (I) 509 | Core paper (Industrial Training, IT) | -- | 5 | 5 | 4 | 100 |
| CHE (I) 510 | Dissertation (DISS)/Project Work (PW) | -- | 15 | 15 | 12 | 300 |
| | | 08 | 20 | 28 | 24 | 600 |

For each paper 30 % weightage is given to internal assessment and 70 % for external assessment.

SEMESTER - 3 (Inorganic Chemistry)

CHE(I) 501 Advanced Inorganic Chemistry

Objective:

To provide basic concepts, synthesis, properties and applications of Nanomaterials. The topic of Ion exchange provides the knowledge of synthesis of resins and their properties. To impart basic and advanced concepts of Supramolecular chemistry. An examination of non-covalent interactions and their impact in chemistry. Topics will include self-assembly with special emphasis on supramolecules derived from calix systems, molecular recognition, and their applications for the design and synthesis of nanostructured materials. The topic of MOFs are very new in recent era.

| | | |
|-----------------|---|------------|
| Unit-I | Advances in Nanomaterials Types of nanomaterials, e.g. nanotubes, nanorods, solid spheres, core-shell nanoparticles, Mesoporous materials; General preparative methods for various nanomaterials, Some important properties of nanomaterials: optical properties of metal and semiconductor nanoparticles, magnetic properties, Some special nanomaterials: Carbon nanotubes: Types, synthesis using various methods, growth mechanism, electronic structure; Porous silicon: Preparation and mechanism of porous silicon formation, Factors affecting porous structure, properties of porous silicon; Aerogels: Types of aerogels, Properties and applications of aerogels, Applications of nanomaterials in electronics, energy, automobiles, sports and toys, textile, cosmetics, medicine, space and defense. Environmental effects of nanotechnology | 25% |
| Unit-II | Ion Exchange Synthesis, characterization and properties of Ion exchangers, mechanism of ion exchange: equilibria–Rate Theory, Donnan equilibria, liquid ion exchangers and chelate ion–exchange resins. Separation of metals and non-meals using ion exchangers. Inorganic ion exchangers : The clay minerals, zeolites, heteropolyacid salts, hydrous oxides and insoluble salts and their applications | 25% |
| Unit-III | Basics of Supramolecular Chemistry Definition and development of supramolecular chemistry, Classification of supramolecular Host-Guest compounds, Receptors, coordination and lock and key analogy, Binding constants, Cooperativity and the chelate effect, Preorganisation and complementarity, Thermodynamic and kinetic selectivity and discrimination, Nature of supramolecular interactions, Solvation and hydrophobic effects, Supramolecular concepts and design | 25% |
| Unit-IV | Metal Organic Frameworks | 25% |

| | | |
|--|--|--|
| | Introduction to MOFs, Synthesis of MOFs, Post-synthetic modification of MOFs, Characterization of MOFs, Characterization of MOFs, Application of MOFs as catalysts, nanoreactors, gas storage devices, etc | |
|--|--|--|

Reference Books:

1. Supramolecular Chemistry by Jonathan W. Steed, Jerry L. Atwood, John Wiley & Sons, Ltd.
2. Supramolecular Chemistry: Concepts and Perspectives By Jean-Marie Lehn
3. Core Concepts in Supramolecular Chemistry and Nanochemistry By Jonathan W. Steed, David R. Turner, Karl Wallace
4. Supramolecular Chemistry- Fundamentals and Applications by Katsuhiko Ariga, Toyoki Kunitake Springer
5. C. E. Harland 1994 Ion exchange theory and practice, 2nd edn, Royal society of Chemistry Cambridge.
6. J. Korkisch 1989 Handbook of ion exchange resins, their application to inorganic chemistry CRC Press, Boca Raton FL.
7. Sulabha K. Kulkarni, Nanotechnology-Principles and Practices, Capital Publishing Co., 2007.
8. Polyoxometalate Chemistry From Topology via Self-Assembly to Applications by Michael T. Pope and Achim Müller, Kluwer Academic Publishers, New York.
9. Advances in Inorganic Chemistry by Rudi van Eldik, Lee Cronin-Polyoxometalate Chemistry, 2017, Zoe Kruze.
10. Nanoparticle Technology for Drug Delivery, Ram B. Gupta and Uday B. Kompella, Taylor & Francis.
11. Metal-Organic Frameworks: Applications from Catalysis to Gas Storage edited by Dr. David Farrusseng, Wiley-VCH.

Learning Outcomes: After completing this course, the student shall

1. understand the types, preparation and applications of nanomaterials. The students utilize this knowledge for their research.
2. Understand the types, preparation and applications of ion exchange resins. The students utilize this knowledge for their research.
3. Understand the basic theory, synthesis and importance of Supramolecular chemistry.
4. know the various supramolecular interactions and host-guest chemistry.
5. The course is specifically design to cater the research need of the department of chemistry, Gujarat University (UGC-SAP, Supramolecular Chemistry) and other university nearby Ahmedabad region such as NFSU, PDPU, CUG, IIT-Gandhinagar.
6. know the MOFs and some terminology of MOFs. The students utilize this knowledge for their research.

SEMESTER - 3 (Inorganic Chemistry)

CHE(I) 502 Catalysis and Organometallic Chemistry

Objective:

To provides basic concept of heterogeneous catalysis and organometallic chemistry. The topic of organometallic chemistry includes synthetic and catalytic aspects of main group organometallic compounds, transition metal organometallic compounds, biological and environmental aspects.

| | | |
|-----------------|---|------------|
| Unit-I | Heterogeneous Catalysis: Fundamentals and Applications Introduction, Definition of catalysis, Types of catalysis, Basics of heterogeneous catalysis, advantages of heterogeneous catalysis, supports for heterogeneous catalysis, Catalytic process, Aspects of heterogeneous catalysis in green chemistry, Applications of heterogeneous catalysis | 25% |
| Unit-II | Synthetic and catalytic aspects of main group organometallic compounds Synthetic applications of main group organometallic compounds as stoichiometric reagents—organolithium, organosodium, organopotassium, organomagnesium, organozinc, organocadmium, organomercury, organoboranes, organoaluminium, organothalium, organosilicon and organotin, Catalytic applications of main group organometallic compounds | 25% |
| Unit-III | Transition metal organometallic compounds as catalysts and synthetic reagents Catalytic processes involving transition metal organometallic compounds as homogeneous catalysts – hydrogenation, hydroformylation, oxidation, isomerization, dimerization and polymerization of alkenes and alkenes metathesis, Catalytic processes based on carbon monoxide and transition metal organometallic compounds as catalysts, Mechanism of reactions catalyzed by transition metal organometallics, Applications of transition metal organometallic compounds as synthetic reagents | 25% |
| Unit-IV | Biological application and environmental aspects of organometallic compounds Introduction, Organometallics in medicine, Organometallics in agriculture and horticulture, Organometallics in industry, environmental aspects of organometallic compounds. | 25% |

Reference Books:

1. Modern Heterogeneous Catalysis by Rutger A. van Santen, Wiley-VCH.
2. Heterogeneous Catalysis: Fundamentals and Applications by Julian R.H. Ross, Elsevier.
3. Handbook of Green Chemistry, Green Catalysis, Vol. 2 by Paul T. Anastas, Wiley-VCH.

4. Organometallic Compounds, Vol.1 & 2 by G.E. Coates, M.L.H. Green and K. Wade, Methuen & Co. Ltd. London EC4.
5. Organometallic Compounds by G.E. Coates, John Wiley & Sons, Inc., New York.
6. Organometallic Chemistry by H. Zeiss, Reinhold Publishing Corporation, New York.
7. Organometallic Chemistry by R.C. Mehrotra & Anirudh Singh, New Age International (P) Limited, Publishers, New Delhi.
8. Progress in Inorganic Chemistry, Vol. 1 by F.A. Cotton, Interscience, Pub.Inc., New York.
9. Organotransition Metal Chemistry by John F. Hartwing, University Science Books, Sausalito, California.

Learning Outcomes: After completing this course, the student shall

1. understand the fundamentals and applications of heterogeneous catalysis. The students utilize this knowledge for their research.
2. Understand the preparation and applications of main group OMC.
3. Understand the basics of catalysis and different catalytic reactions promoted by OMC and importance of OMC.
4. know the biological and environmental aspects of OMC.
5. The course is specifically design to cater the research need of the department of chemistry, Gujarat University and other university nearby Ahmedabad region such as NFSU, PDP, CUG, IIT-Gandhinagar.

SEMESTER - 3 (Inorganic Chemistry)

CHE(I) 503 Spectroscopy

Objective:

The main objective of the course is to make students aware of theoretical aspect of different spectroscopic techniques such as IR, UV, NMR, ESR and mass spectroscopy. Objective is to understand the principles, instrumentation and applications of FT-IR and UV. Objective is to understand the principles, instrumentation, some important terms and applications of ^1H & ^{13}C -NMR. Objective is to understand the principles, instrumentation and applications of ESR. Understanding of concepts of Double Resonance and Fourier transform EPR techniques. Mossbauer spectroscopy and microscopic techniques such as SEM, STF, AFM. Objective is to understand the principles, instrumentation, some important terms and applications of all the techniques. Final objective is to learn structure elucidation of unknown compounds.

| | | |
|-----------------|---|------------|
| Unit-I | Infrared Spectroscopy: Theory and Application of FT-IR. Symmetry and shape of AB_2 , AB_3 , AB_4 , AB_5 and AB_6 . Modes of bonding of ambidentate ligands. Effect on coordination on ligand Bands, Change in symmetry on coordination. Organometallic compounds. Metal ligand vibration. Ultraviolet Spectroscopy Theory of electronic transition and auxochromes, Woodward-Fieser rules, Characteristic absorptions in various compounds | 25% |
| Unit-II | Nuclear Magnetic Resonance Spectroscopy ^1H Nuclear Magnetic Resonance (^1H NMR) spectroscopy, Chemical shifts and factors affecting chemical shifts, Splitting of the signals – spin couplings and coupling constants, Chemical shift equivalence and magnetic equivalence, ^{13}C -NMR spectroscopy, Proton coupled and decoupled ^{13}C NMR spectra, Chemical shifts in ^{13}C NMR spectra and their calculation, ^{13}C - ^1H coupling constants, ^{13}C -DEPT spectra, Nuclear Overhauser Effect, NMR Spectroscopy of other important spin $\frac{1}{2}$ nuclei, Interpretation of NMR spectra Contact shift and pseudocontact shift. Lanthanide complexes as shift reagents. Double resonance Technique. | 25% |
| Unit-III | Electron Spin Resonance. Theory of Electron Spin Resonance (ESR) Spectroscopy, Instrumentation, Factors affecting the g-values, Differences between NMR and ESR, | 25% |

| | | |
|----------------|---|------------|
| | Hyperfine interactions, Interpretation of ESR spectra, Applications of ESR, Survey of EPR spectra of first row transition metal ion complexes, Double Resonance and Fourier transform EPR techniques. | |
| Unit-IV | <p>Mossbauer Spectroscopy and Microscopic Techniques:</p> <p>(a) Mossbauer Spectroscopy Basic principle, Spectral parameters and spectrum display. Interpretation of Isomer shift. Application of Technique to the studies of bonding and structure of Fe²⁺ and Fe³⁺ compounds, Sn²⁺ and Sn⁴⁺ compounds and detection of oxidation states. FAB and electrospray mass spectrometry of metal complexes.</p> <p>(b) Microscopic Techniques: Introduction to scanning electron microscopy (SEM), Scanning tunneling microscopy (STM) and atomic force microscopy (AFM); basic principles and theory; instrumentation and operating parameters and applications</p> | 25% |

Reference Books:

1. Spectroscopic Identification of Organic Compounds by R. M. Silverstein and F. X. Webster, 6th edition, John Wiley & Sons.
2. Introduction to Spectroscopy by D. L. Pavia, G. M. Lampman and G. S. Kriz, 3rd edition, Thomson Brooks/Cole.
3. Spectroscopic Methods in Organic Chemistry by D. H. Williams and I. Fleming, 4th edition, Mcgraw–Hill Book Company.
4. Organic Spectroscopy by William Kemp, 3rd edition, Palgrave.
5. Organic Spectroscopy–Principles and Applications by Jag Mohan, 2nd edition, Narosa Publishing House.
6. Spectroscopy of Organic Compounds by P. S. Kalsi, 5th edition, New Age International Publishers.

Learning Outcomes: After completing this course, the student shall

1. Understand the theory, instrumentation and interpretation of FT-IR and UV.
2. know the principles and some terminology of ¹H & ¹³C - NMR. They are able to used shift reagents.
3. understand the principle, instrumentation and applications of ESR.
4. understand the theory, instrumentation important terms of mass spectrometry.
5. With understanding of all four units, students are able to characterization of molecules, which is helpful for their professional and research carrier.

SEMESTER - 3 (Inorganic Chemistry)

CHE(EI) 504 Applications of Inorganic Chemistry in Industry

Objective:

To impart basic knowledge of Inorganic chemistry in Industry. The course includes introduction, synthesis manufacturing process and applications of some pigments, smart materials, corrosion inhibitors and inorganic polymers. These topics are very important and used in industries.

| | | |
|-----------------|--|------------|
| Unit-I | Pigments Introduction; Pigments in foods–naturally occurring plant- and animal-pigments; Synthetic food pigments such as Sunset yellow, Allura red, etc.; pigments in plants –raw materials for paints; Physical properties of the pigments in paints; Brief descriptions of the manufacturing process and use of commonly used pigments such as White lead, Zinc oxide, Titanium dioxide, etc. | 25% |
| Unit-II | Smart materials Ceramics, alloys, gels and polymers. Piezoelectric materials, electrostrictive and magnetostrictive materials, rheological, thermoresponve, pH sensitive halochromic materials, electrochromic materials and smart gels. | 25% |
| Unit-III | Corrosion Inhibitors Introduction, Types of corrosion Principles of corrosion inhibitors, corrosion as an electrochemical process, Practical aspects of corrosion inhibition, Anion inhibitor properties in neutral electrolytes, some application of corrosion inhibitors (cooling water circulation-once through and open systems, engine radiation & cooling systems, central heating system, refrigeration plants and high chloride systems, water for steam raising, corrosion inhibitors for paint coating plastic linings, alloying for corrosion resistance) | 25% |
| Unit-IV | Inorganic Polymers Introduction, Classification of inorganic polymers, General properties of inorganic polymers, Characterization of inorganic polymers, Crystalline and amorphous polymers, Solubility parameter, Glass-transition temperature, Modulus-temperature curves, Important inorganic polymers: phosphorus-based polymers, Sulphur-based polymers, Boron-based polymers, Silicon-based polymers, Pre-ceramic Inorganic polymers | 25% |

Reference Books:

1. UHLIGS Corrosion Handbook, R. Winston Revie., Jhon Wiley & Sons JNC.
2. An Introduction to metallic corrosion, U.R. Evans, Cambridge, England.

3. Handbook of Industrial Chemistry, Vol.1 by K.H.Davis, F.S.Berner, CBS Publishers, Bangalore.
4. Comprehensive Coordination Chemistry, Chapter 57, 58.
5. Insight into Speciality Inorganic Chemicals, Chapter 15, by David Thompson, The Royal Society of Chemistry, 1995.
6. New Trends in Green Chemistry, 2nd Edition by V.K.Ahluwalia and M.Kidwai, Anamaya Publishers, 2007.
7. Advanced Inorganic Chemistry Vol. 1, Gurdeep Raj, Krishna Publication Meerut.
8. Inorganic Polymers, 2nd Edition by J.E. Mark, H.R. Allcock, R. West, Oxford University Press, Inc., New York.
9. Inorganic and Organometallic Polymers by R.D. Archer, Wiley-VCH, Inc.
10. Inorganic Polymers by D.N. Hunter.
11. Modern Aspects of Inorganic Chemistry by H.Emeleus and A.G.Sharpe, Universal Books Stall, New Delhi Routledge & Kegan paul, London.
12. Inorganic Polymers by G.R.Chatwal, Himalaya Publishing House.

Learning Outcomes: After completing this course, the student shall

1. Understand the importance of pigments and their synthesis.
2. know the smart material and applications.
3. understand the types, preparation and applications of corrosion inhibitors. The students utilize this knowledge for their research.
4. Knowledge of coordination polymers open the opportunities in related industries in the state of Gujarat. Which is helpful for their professional and research carrier.
5. With understanding of all four units, students easily absorb in the chemical industries.

SEMESTER - 3 (Inorganic Chemistry)

CHE(EI) 504 Spectroscopy-II

Objective:

The main objective of the course is to make students aware of theoretical aspect of different analytical instrumentation techniques such as thermal methods, X-ray diffraction methods, Electron spectroscopy such as XPS, UPS, AES, Atomic absorption and Flame Emission spectroscopy. Objective is to understand the principles, instrumentation and applications of mass spectrometer, the use of ionization techniques based on application, the basic concepts of Fragmentation Rules and its applications. Final objective is to learn structure elucidation of unknown compounds.

| | | |
|-----------------|--|------------|
| Unit-I | Thermal and X-ray diffraction methods (a) Thermal methods: Principles, instrumentation and application of TGA, DTA and DSC. (b) X-ray diffraction Methods: Production of x-rays and Bragg's equation, instrumentation and application for structural studies | 25% |
| Unit-II | Electron Spectroscopy: Introduction, principle and theory of electron spectroscopy, Notations, X-ray Photoelectron Spectroscopy (XPS), Ultraviolet Photoelectron Spectroscopy (UPS), Auger Electron Spectroscopy (AES), Instrumentation of electron spectroscopy, Qualitative and Qualitative analysis by electron spectroscopy, Chemical shifts, Unwanted features in electron spectra, Applications of electron spectroscopy | 25% |
| Unit-III | Atomic Absorption/Atomic and Flame Emission Spectroscopy Absorption of radiation by atoms; equipment: radiation sources (Hollow cathode lamps and electrode less discharge lamps); atomizers (Flame and carbon); wavelength selector and detectors; interferences in atomic absorption spectroscopy; applications and problems: qualitative and quantitative analysis. Introduction to plasma, arc and spark emission spectroscopy; equipment: inductively coupled plasma spectrometer and flame photometer; applications and problems | 25% |
| Unit-IV | Mass Spectroscopy Theory of Mass Spectroscopy, Instrumentation, Ionization techniques, Mass analyzers, Fragmentations and rearrangements, Interpretation of mass spectra, Determination of molecular formula, Mass spectra of some chemical classes | 25% |

Reference Books:

1. Elements of X-Ray Diffraction (3rd Edition), B.D.Cullity,
- 2.“Principles and Practice of X – Ray Spectrometric Analysis”, 2nd edition, Bertin, Eugene, Plenum Press, New York, 1975.
- 3.“An Introduction to X –Ray Spectrometry”, Jenkins, Ron, Heyden & Sons, London, 1974.
4. Principles of Instrumental Analysis” by Douglas A. Skoog, 3rd Edition, Holt-Saunders International Edition
5. Principles of Instrumental Analysis by Skoog, Holler and Neiman, Sanders College Publishers (USA).
6. Undergraduate Instrumental Analysis by James W. Robinson, Marcel Dekker, Inc. (Ny.)
7. Introduction to Instrumental Analysis by Robert D. Braun, Pharme Med Press Hyderabad-India.
8. Instrumental Method of Analysis by Willard, Merritt, Jr., Dean and Settle Jr., CBS Publishers and distributors, New Delhi, India.
9. Microscopic and Spectroscopic Imaging of the Chemical State by Michael D. Morris, Marcel Dekker, Inc. (NY.).
- 10.Instrumental Methods of Chemical Analysis, 24th Edition 2005 by B. K. Sharma, Goel Publishing House, Meerut

Learning Outcomes: After completing this course, the student shall

1. Understand the theory, instrumentation and important terms of TGA and XRD.
2. know the principles and instrumentation and applications of XPS, UPS, AES.
3. understand the principle, instrumentation and applications of AAS.
4. understand the theory, instrumentation important terms of mass spectrometry.
5. With understanding of all four units, students are able to characterization of molecules, which is helpful for their professional and research carrier.

SEMESTER - 3 (Inorganic Chemistry)

CHE(EI) 504 Transition Metal Organometallic Chemistry: Principles to Applications (*Online through SWAYAM*)

Transition Metal Organometallic Chemistry: Principles to Applications

By Prof. P. Ghosh | IIT Bombay https://onlinecourses.nptel.ac.in/noc21_cy36/preview

This course would cover all aspects of Organometallic Chemistry, starting from the principles to its applications.

INTENDED AUDIENCE: All of Chemistry and possibly some of Chemical Engineering students.

PREREQUISITES: UG General Chemistry.

INDUSTRY SUPPORT: Reliance, Dupont, BASF, BAYER, DOW Chemicals.

| Summary | |
|-------------------|----------------------------|
| Course Status : | Upcoming |
| Course Type : | Elective |
| Duration : | 12 weeks |
| Start Date : | 26 Jul 2021 |
| End Date : | 15 Oct 2021 |
| Exam Date : | 24 Oct 2021 |
| Enrollment Ends : | 02 Aug 2021 |
| Category : | o Chemistry |
| Credit Points : | 3 |
| Level : | Undergraduate/Postgraduate |

This is an AICTE approved FDP course

Course layout

Week 1 :

Lecture 1: History of Organometallic Compounds,

Lecture 2: Polarity and Reactivity of M–C bond

Lecture 3: Reactivity of Organometallic Compounds

Lecture 4: Reactivity of Organometallic Compounds (contd...)

Lecture 5: 18 Valence Electron Rule and Classification

Week 2 :

Lecture 6: 18 Valence Electron Rule and Classification

Lecture 7: Reactivity and types of Organometallic compounds

Lecture 8: sigma- Donor ligands

Lecture 9: Preparation of sigma- alkyl compounds

Lecture 10: Preparation and Properties of sigma- alkyl compounds

Week 3 :

Lecture 11: Properties of sigma- alkyl compounds

Lecture 12: β -elimination in sigma- alkyl compounds

Lecture 13: β -elimination in detail

Lecture 14: TM sigma- alkyl complexes and its application

Lecture 15: TM sigma- alkyl complexes and its application (contd...)

Week 4 :

Lecture 16: C-H activation

Lecture 17: C-H activation in details

Lecture 18: C-H activation in details (contd...)

Lecture 19: Characterization of C-H activation

Lecture 20: Bonding in C-H activation

Week 5 :

Lecture 21: C-C Bond activation

Lecture 22: C-C Bond activation (contd...)

Lecture 23: C-C Bond activation in Details

Lecture 24: Transition Metal Perfluoroalkyl (RF-TM) Complexes

Lecture 25: Preparation of Transition Metal Perfluoroalkyl (RF-TM) Complexes

Week 6 :

Lecture 26: C-F Activation

Lecture 27: Transition Metal Alkenyl/Aryl Complexes

Lecture 28: Transition Metal Aryl Complexes

Lecture 29: Transition Metal Aryl/Alkyne Complexes

Lecture 30: Transition Metal Alkyne/Carbene Complexes

Week 7 :

Lecture 31: Transition Metal Carbene Complexes: Preparations

Lecture 32: Transition Metal Carbene Complexes: Properties

Lecture 33: Transition Metal Carbene Complexes: Reactivities

Lecture 34: Transition Metal Carbene Complexes: Reactivities (contd...)

Lecture 35: Transition Metal Carbene Complexes: Reactivities (contd...)

Week 8 :

Lecture 36: Transition Metal Carbene Complexes: Reactivities (contd...)

Lecture 37: Reactivity of Schrock type Carbene Complexes and Transition Metal Carbynes

Lecture 38: Transition Metal Carbynes: Preparation

Lecture 39: Transition Metal Carbynes: Properties

Lecture 40: Transition Metal Carbynes: Properties (contd...)

Week 9 :

Lecture 41: Properties of Transition Metal Carbynes And Transition Metal Carbonyls

Lecture 42: Transition Metal Carbonyls

Lecture 43: Transition Metal Carbonyls (contd...)

Lecture 44: Transition Metal Carbonyls: Bonding properties

Lecture 45: Transition Metal Carbonyls: Bonding properties (contd...)

Week 10 :

Lecture 46: Transition Metal Carbonyls: Reactivities

Lecture 47: Transition Metal Carbonyls: Reactivity and Carbonyl Metallates

Lecture 48: Transition Metal Carbonyl Hydrides

Lecture 49: Application of Carbonyl Metallates and Metal Halides

Lecture 50: Application of Metal Halides and Metal Alkenes

Week 11 :

Lecture 51: Transition Metal Olefin Complexes

Lecture 52: Transition Metal Olefin Complexes (contd...)

Lecture 53: Transition Metal Olefin Complexes: Reactivity

Lecture 54: Bonding Properties in Olefin Complexes

Lecture 55: Transition Metal Diolefin Complexes

Week 12 :

Lecture 56: Transition Metal Diolefin and Alkyne Complexes

Lecture 57: Transition Metal Alkyne Complexes

Lecture 58: Transition Metal Alkyne Complexes: Reactivity

Lecture 59: Transition Metal Alkyne Complexes: Reactivity (contd...)

Lecture 60: Summary: Transition Metal Organometallic Chemistry: Principles to Applications

Books and references

Elschenbroich (Organometallics), Crabtree (Organometallics)

Instructor bio

Prof. P. Ghosh

IIT Bombay

Dr. Prasenjit Ghosh is a Professor of Inorganic Chemistry at Indian Institute of Technology Bombay (IIT Bombay), India. He received his PhD in bioinorganic chemistry under the supervision of Professor Gerard Parkin from Columbia University, New York, in 1998. Following two post- doctoral stints in the laboratories of Dr. R. Morris Bullock (Brookhaven National Laboratory, 1998-2001) and Professor Guillermo C. Bazan (University of California, Santa Barbara, 2001-2003), he joined the Department of Chemistry at IIT Bombay as an Assistant Professor in 2003 and was finally promoted to Professor in June, 2012. He received the CRSI Bronze Medal (2014) of the Chemical Research Society of India and The Distinguished Lectureship Award (2011) of the Chemical Society of Japan among many others in the recent

years. He is an Editorial Advisory Board member of the ACS journal Organometallics from 2017 for a three-year period and of Polyhedron since 2011.

Course certificate

The course is free to enroll and learn from. But if you want a certificate, you have to register and write the proctored exam conducted by us in person at any of the designated exam centres.

The exam is optional for a fee of Rs 1000/- (Rupees one thousand only).

Date and Time of Exams: **24 October 2021** Morning session 9am to 12 noon; Afternoon Session 2pm to 5pm.

Registration url: Announcements will be made when the registration form is open for registrations.

The online registration form has to be filled and the certification exam fee needs to be paid. More details will be made available when the exam registration form is published. If there are any changes, it will be mentioned then.

Please check the form for more details on the cities where the exams will be held, the conditions you agree to when you fill the form etc.

CRITERIA TO GET A CERTIFICATE

Average assignment score = 25% of average of best 8 assignments out of the total 12 assignments given in the course.

Exam score = 75% of the proctored certification exam score out of 100

Final score = Average assignment score + Exam score

YOU WILL BE ELIGIBLE FOR A CERTIFICATE ONLY IF AVERAGE ASSIGNMENT SCORE $\geq 10/25$ AND EXAM SCORE $\geq 30/75$. If one of the 2 criteria is not met, you will not get the certificate even if the Final score $\geq 40/100$.

Certificate will have your name, photograph and the score in the final exam with the breakup. It will have the logos of NPTEL and IIT Bombay. It will be e-verifiable at nptel.ac.in/noc.

Only the e-certificate will be made available. Hard copies will not be dispatched.

Once again, thanks for your interest in our online courses and certification. Happy learning.

- NPTEL team

SEMESTER - 3 (Inorganic Chemistry)

CHE(I) 505 & 506 PR(PRACTICALS)

Objective:

To impart practical knowledge and skills in inorganic laboratories and synthesis and characterization of various complexes and compounds using modern instrumental techniques. Analysis of alloys, industrial waste and cement includes understandings of standardization of various reagents, buffer solution preparation, decomposition of material etc.

CHE(I) 505 PRACTICALS: Synthesis of inorganic complexes/compounds and their characterization by various physicochemical methods, viz. IR, UV, Visible, NMR, magnetic susceptibility etc. Selection can be made from the following or any other from the existed literature.

1. Cis and trans isomers of $[\text{Co}(\text{en})_2\text{Cl}_2]\text{Cl}$
J. Chem. Soc., 1960, 4369.
2. Ion-exchange separation of oxidation states of vanadium.
J. Chem. Educ., 1980, 57, 316; 1978, 55, 55.
3. Preparation of Ferrocene.
J. Chem. Educ. 1966, 43, 73; 1976, 53, 730.
4. Preparation of triphenyl phosphine PPh_3 , and its transition metal complexes.
5. Determination of Cr(III) complexes.
 $[\text{Cr}(\text{H}_2\text{O})_6]\text{NO}_3 \cdot 3\text{H}_2\text{O}$; $[\text{Cr}(\text{H}_2\text{O})_4\text{Cl}_2]\text{Cl} \cdot 2\text{H}_2\text{O}$; $[\text{Cr}(\text{en})_3]\text{Cl}_3$; $\text{Cr}(\text{acac})_3$
6. Tin(IV) iodide, Tin(IV) chloride, Tin(II) iodide
Inorg. Synth. 1953, 4, 119
7. (N,N)-bis(salicylaldehyde)ethylenediamine SalenH_2 ; and its cobalt complex $[\text{Co}(\text{Salen})]$.
J. Chem. Educ., 1977, 54, 443; 1973, 50, 670.
8. Vanadyl acetylacetonate
9. Reaction of Cr(III) with multidentate ligands, a kinetics experiment.
J. Am. Chem. Soc., 1953, 75, 5670.
10. Mixed valence dinuclear complex of Manganese(III, IV).
11. Other new novel synthesis reported in literature time to time.

CHE(I) 506 PRACTICALS: Alloys analysis, Ion exchange, complexometry, industrial waste and cement

1. Analysis of BRONZE
2. Analysis of Solder
3. Analysis of Steel
4. Analysis Aluminum alloy
5. Analysis of Gun metal
6. Capacity of ion exchangers
7. Separation of cations and anions using ion exchangers (3)
8. Analysis of mixtures by complexometry (3)
9. Analysis of Industrial waste
10. Determination of Calcium fluoride, Calcium and Carbonate from Industrial waste
11. Analysis of Cement: (White/Black Cement). Determination of SiO_2 , Fe^{+3} , Al^{+3} , Ca^{+2} , Mg^{+2} in a given sample.

Reference Books:

1. Qualitative Chemical semimicroanalysis by V. N. Alexeyev, Mir Publishers Moscow.
2. Vogel's Qualitative Inorganic Analysis by G. Svehla, Orent Longman, New Delhi.
3. Vogel's Textbook of Quantitative Chemical Analysis, 5th edition by G. H. Jeffery, J. Bassett, J. Mendham and R. C. Denney, ELBS Publication, 1996, Chapter 2, 3, 11.
4. Modern Analytical Chemistry, 1st Edition by D. Harvey, The McGraw-Hill Pub, 2000.
5. Instrumental Methods of Analysis, 4th edition by G.W. Ewing, McFraw Hill Ltd., 1970.
6. Physical Methods in Inorganic Chemistry by R. S. Drago, John-Wiley Pub., 1975.

Learning Outcomes: After completing this course, the student shall

1. Understand the synthesis of various complexes.
2. know the practical applications of coordination chemistry, various instrument and characterization.
3. understand the types and applications of ion exchange resins. The students utilize this knowledge for their research.
4. Knowledge of cement and waste analysis allow student to absorb in chemical industries

SEMESTER – 4 (Inorganic Chemistry)

CHE(I) 507 Scientific Writing

- ♦ Writing of Research Article/Review Article/Commentary Article/Case Study/Monograph/Book Chapter/Book Review/Research Proposal or any other scientific article type.
- ♦ The student can select any one scientific writing type or research proposal and submit a copy (hard and soft) of the same for internal and external evaluation.
- ♦ Evaluation shall be centered around on novelty, relevance, significance, and impact.
- ♦ Additional weightage will be given for submission/publishing of any article type in any journal (University journal or a journal that is indexed in the UGC CARE list/Web of Science/ SCOPUS/SCI/SCIE etc.) or a research proposal.

Guidelines for Scientific Writing

Research Article

Presents a full report with new results on a specific topic. Complete experimental details with proper justification. Generally not limited in length, with figures, tables, and references. Format...Title, Authors, Abstract, introduction, experimental, results, discussion, conclusion, acknowledgment, references

Review Articles/Commentary Article

Gives an overview of research in a particular field. It can be on one's own research or any other topic of general and current interest. Organized differently from communications or research articles as it does not have primary experimental data.

Data of existing literature can be presented in a tabular format, graphs, diagrams, figures, charts etc. Should be referenced as thoroughly as possible. Format...Title, Authors, Abstract, introduction, discussion, conclusion, acknowledgment, references

Case Study

This study represents person, group, or situation that has been studied over time. Format depends upon the type of study.

Monograph

Title, Author, Introduction: Reason to select a topic; History, timeline, and Scientific/social significance; Benefits to the scientific community, teaching, and research, Development: Exposition of ideas into paragraphs or chapters.

“Quote that authors endorse these ideas.” Conclusion: Status and future perspectives, References: Should be referenced as thoroughly as possible

Book Chapter

Title, Authors, Abstract, Introduction/Background on the topic, Discussion (with subdivisions): Text with tables, figures, charts etc., Summary/Conclusion: Status and future perspectives, References

Book Review

A book review is a thorough description, critical analysis, and/or evaluation of the quality, meaning, and significance of a book, often written in relation to prior research on the topic. Scope/Purpose/Content, Note the Method/Methodology of writing, Critically Evaluate the Contents, Examine the Front Matter and Back Matter, Summarize and Comment.

Research Proposal

Title, Research Problem/Problem Statement, Rational/Purpose of the Study, Review of the Literature, Proposed Research Framework, Research Questions/Proposed Hypothesis, Significance, Proposed Methods and Procedures, Deliverables/Expected Outcomes, Execution timelines, year wise breakup, Financial aspects, References

References

- 1 “*A Manual for Writers of Research Papers, Theses, and Dissertations*”, Kate Turabian, University of Chicago Press, 8th Edition, 2013.
- 2 “*Concise Guide to Writing Research Papers (Perfect Phrases Series)*”, Carol Ellison, McGraw-Hill Education; 1st Edition, 2010.

SEMESTER – 4 (Inorganic Chemistry)

CHE(I) 508 Report Writing

- ◆ Report Writing for Participation and/or presentation (Poster/Oral/Invited talk as applicable) in University/State level/National/International Seminar/ Conference/Webinar/ Symposium/Workshop/Hands-on training/Software learning of at least 2 days. In case of one day seminar/ webinar/ conference/workshop, it is mandatory to participate in two such events.
- ◆ Evaluation will be based on detailed technical report prepared on the conference/seminar/workshop participated and for Poster/Oral presentation, as applicable.
- ◆ Additional weightage will be given for Poster/Oral presentations.

Guidelines for Report Writing

It aims to summarise the most important talks/research presented. It is not usually feasible to attempt comprehensive coverage of the conference. More focus should be on those presentations that are most topical, interesting, or thought-provoking.

Points to consider when writing the report:

- Name of Institute/Department/University that organized the conference
- Title and theme of the conference
- Information regarding number of attendees, where and when it was held (date), name of the convener, organizing secretary etc.
- Include a copy of the brochure
- A brief about the Inaugural Session
- Details of all the technical sessions
- List of main speakers, their position/designation, topic, expertise, and their institutional affiliation
- Highlight research paper(s) or work with major significance and impact
- A brief about the Concluding/Valedictory Session
- Embed the text with photographs wherever possible
- The outcome/summary: Your learning

References

- 1 “*Writing for Conferences: A Handbook for Graduate Students and Faculty*”, Leo Mallette, Clare Berger, Greenwood; Illustrated Edition, 2011.
- 2 “*The Creative Writing Handbook*”, John Singleton (Editor), Mary Luckhurst (Editor), Red Globe Press; 2nd Edition, 1999.

SEMESTER – 4 (Inorganic Chemistry)

CHE(I) 509 Industrial Training

Guidelines for Industrial Training

- 1 Each student must undergo 3 weeks industrial training under the supervision of a faculty from the concerned department.
- 2 The industry may be in Ahmedabad, Gujarat or anywhere in India.
- 3 The training may be obtained at any R&D, QA, QC, Production or any other relevant department on different instrumental techniques or other laboratory equipments.
- 4 The students must submit a report on the training obtained from the industry which may include (a) introduction about the industry (b) various activities of the industry (c) the process which are used in the industry (d) the products of the industry and (e) summary and conclusion.
- 5 The report submitted by each student would be assessed by the branch in-charge and the supervising teacher.
- 6 The student must discuss/present the details of the training through a power point presentation

SEMESTER – 4 (Inorganic Chemistry)

CHE(I) 510 Dissertation

Guidelines for Dissertation/Project Work

- 1 Each student must carry out a project under the supervision of a faculty from the concerned department.
- 2 The project can be carried out either in the department or in any other industry, institute or organizations located in Ahmedabad, Gujarat or anywhere in India.
- 3 The topics of the dissertation can be selected from any of the four branches of chemistry i.e., Organic, Inorganic, Physical or Analytical. The topic can be related to (a) synthesis, purification, characterization, application of organic compounds or (b) metal complexes preparation and applications or (c) physical studies of various systems (d) method development and validation (e) green chemistry (f) nanomaterials preparation and applications (g) functionalized supramolecules (h) electro analytical methods (i) environmental analysis and decontamination or any other related to the subject.
- 4 Each student must submit a dissertation on the topic of their study comprising of (a) an introduction on the topic along with literature survey and justification for the selection of the topic (b) materials and methods (c) methodology (d) results and discussion and (e) summary and conclusion along with the references.
- 5 Each student must give monthly report and a midterm presentation of their work at the department.
- 6 The student must discuss/present the details of dissertation through a power-point presentation.
- 7 Dissertation would be examined by the supervising teacher and external examiner.

GUJARAT UNIVERSITY
MSc Organic Chemistry Semester III and IV
Revised Syllabus
Design and Structure of Choice Based Credit System
(Effective from 2021-2022)

| MSc Semester III | | | | | | |
|------------------|--|---|-------------------|-----------|------------------|------------|
| Course | | No. of hours per week (12 h for each unit and 48 h for each paper/course) | | | Total credits | Marks |
| Paper Code | Type | Lectures | Labs | Total | | |
| CHE (O) 501 | Core Paper | 4 | -- | 4 | 4 | 100 |
| CHE (O) 502 | Core Paper | 4 | -- | 4 | 4 | 100 |
| CHE (O) 503 | Core Paper | 4 | -- | 4 | 4 | 100 |
| CHE (EO) 504 | Elective Paper | 4 | -- | 4 | 4 | 100 |
| CHE (O) 505 PR | Lab Course 1 | -- | 6 | 6 | 4 | 100 |
| CHE (O) 506 PR | Lab Course 2 | -- | 6 | 6 | 4 | 100 |
| | Total | 16 | 12 | 28 | 24 | 600 |
| MSc Semester IV | | | | | | |
| Course | | No. of hours per week (12 h for each unit and 48 h for each paper/course) | | | Total credits | Marks |
| Paper Code | Type | Lectures/ Discussion | DISS/PW and IT | Total | | |
| CHE (O) 507 | Core Paper (Scientific Writing) | 4 | -- | 4 | 4 | 100 |
| CHE (O) 508 | Core Paper (Report Writing) | 4 | -- | 4 | 4 | 100 |
| CHE (O) 509 | Core paper (Industrial Training, IT)/NET-GSET based Test | -- | 5 | 5 | 4 | 100 |
| CHE (O) 510 | Dissertation (DISS)/Project Work (PW) | -- | 15 | 15 | 12 | 300 |
| | | 08 | 20 | 28 | 24 | 600 |

For each paper 30 % weightage is given to internal assessment and 70 % for external assessment.

CHE(O) 501 Natural Products and Bio molecules

Learning objective:

1. To understand the concept of biomolecules and natural product.
2. To understand the natural and synthetic pathways of the biomolecules and natural product.

Learning Outcomes

1. Learner can understand different types of steroids and hormones.
2. From Protein and peptides students will learn the topic and understand the importance of the same.
3. Study of different types of carbohydrates and their structures.
4. Students will learn the importance of nucleic acid in the DNA, RNA and proteins.

Unit I: Steroids and hormones

Introduction, Biogenesis of Steroids, Chemistry of cholesterol and ergosterol (no synthesis), Chemistry and synthesis of sex hormones (Testosterone, Oestrone, Progesterone) from cholesterol, Partial synthesis of Cortisone, Chemistry of bile acids, Plant hormones (auxins, heteroauxins, gibberellins)

Unit – II -Protein and peptides

Introduction of protein, Stereoisomerism in α -amino acid, Acid-base properties of amino acid, Isoelectric Points and Electrophoresis, Reductive Amination, Structure and nomenclature of peptides, Classification of amino acids, Disulfide linkages in peptides, Amino acids sequence determination in polypeptide, Modern synthetic approach for end group analysis, Solution-phase peptide synthesis, Solid-phase peptide synthesis

Unit – III-Carbohydrates

Introduction & definition, Classification, Types of glycosidic linkage, Chemistry of cellulose, Chemistry of starch, Chemistry of glycogen, Configuration of monosaccharides, Ring structure of monosaccharides, Disaccharides, Derivatives of polysaccharides

Unit – IV -Nucleic acid and Fatty acid

Compounds of nucleic acids, nomenclature of nucleotides, nucleosides, structure of DNA & chemical parameters, DNA, proteins, structure of RNA, chemical synthesis of purine nucleobases, Prebiotic chemistry, Synthesis of nucleosides, Chemistry of polymerase chain reaction, DNA sequencing: Sanger's di-deoxy method, Fatty acids, saturated fatty acids, unsaturated fatty acids, essential fatty acids

Reference books:

1. Organic chemistry vol. I & II (sixth edition) I. L. Finar
2. Organic chemistry of natural products (Volume-1), Gurdeep R. Chatwal, Himalaya Publishing House
3. Chemistry of Natural products vol I & II by O.P.Agrawal
4. Chemistry of vitamins-S. F. Dyke
5. Chemistry of natural products by Bantely, Vol 1-10
6. Organic chemistry, L. J. Wade Jr., Prentice Hall, Englewood Cliffs, 1987

CHE(O) 502 **Advanced organic synthesis**

Learning objective:

3. To understand the reaction mechanism of a chemical reaction, the path and the feasibility of a reaction.
4. To suggest synthetic route for complex organic compounds with stereochemistry.
5. To understand the techniques involved in the determination of mechanism of reacted ions and to propose methods to determine the mechanism of reaction.
6. To make the students understand and appreciate the concept of Stereochemistry and reaction mechanism.

Learning Outcomes

5. Learner can understand deep aspects of retrosynthesis and oxidation-reduction reaction.
6. Learner can understand synthesis of the important organic molecule.
7. Learner can be able to design new molecules of interest.
8. PCR and Conformational analysis can give understanding of how the reactions take place by bond shifting and geometry.
9. Protection groups concept is important to synthesized desired compounds to avoid side reaction/products during organic synthesis.

Unit-I- PCR and Conformational analysis

Introduction & classification, Electrocyclic reactions - introduction, definition and classification, Woodward-Hoffmann rules for electrocyclic reactions, Stereochemical aspects and modes of electrocyclic reactions, Cycloaddition reactions, Woodward- Hoffmann rules for cycloaddition reactions, Examples of thermal and photochemical [2p+2p] cycloaddition reactions, 1,3-Dipolar cycloaddition reactions, higher order cycloaddition reactions, Sigmatropic rearrangements - examples, Claisen and Cope rearrangements, Conformation and Configuration, Barriers to rotation, Conformation of ethane, propane, butane, Ring strain, Ring inversion of cyclohexane, Substituted cyclohexane, Decalins

Unit-II- Protecting groups

Role of protecting group in organic synthesis, principle of protection of hydroxyl (alcohol and phenol), amino [amine – (primary, secondary) and amide], carbonyl (ketone and aldehyde), carboxylic acid with different (minimum 5) reagents and their deprotection, synthetic equivalent groups (application of protection & deprotection approach with proper organic reaction).

Unit-III Retrosynthesis

Introduction and terminology, guidelines for disconnections, functional group inter- conversions, the importance of the order of events in organic synthesis, chemo selectivity, one group C-X and two group C-X disconnections, Natural reactivity' and 'umpolung', (epoxide, Haloketones and esters, 1,3 dithiane, cyanide, Nitro, alkynes) C-C disconnection: Introduction, Alcohols, and carbonyl compounds, regioselectivity, alkene synthesis, use of acetylenes and aliphatic nitro compounds in organic synthesis.

Unit IV: Oxidation-Reduction

Oxidation: Introduction, oxidation of hydrocarbons (alkanes, alkenes, aromatic ring), phenol, alcohols and diols, ketones (aldehydes, carboxylic acids and their derivatives), amines, hydrazine and sulphides.

Reduction: Introduction, reduction of hydrocarbons (alkenes, alkynes, aromatic ring), ketones (aldehydes, carboxylic acids and their derivatives, esters), anhydrides, nitrile, epoxides, nitro, nitroso, azo and oxime groups

Reference:

1. T. W. Greens, P. G. M. Wuts. Protective groups in Organic synthesis, 3rd / 4th Ed. John Wiley & Sons, INC
2. Organic chemistry- Clayden, Greeves, Warren and Wothers
3. Advance organic chemistry by Jerry March
4. Advance organic chemistry by Carey and Sundberg,
5. Advance organic chemistry by Francis A. carey
6. Designing Organic Synthesis, S. Warren, Wiley.
7. Organic Synthesis- Concept, Methods and Starting Materials, J. Fuhrhop and G. Penzillin, Verlage VCH.
8. Some Modern Methods of Organic Synthesis, W. Carruthers, Cambridge Univ. Press.
9. Handbook of Reagents for Organic Synthesis - Oxidizing and Reducing Agents
Burke, Steven D., Danheiser, Rick L. (Eds.)

CHE(O) 503 Organic spectroscopy

Course Objectives:

1. To familiarize students with the most commonly used spectroscopic techniques.
2. Introduce basic and essential requirements to solve or understand the spectral problem.
3. Develop basic skills to interpret the spectra using spectroscopic data
4. To understand the basic spectroscopy of organic chemistry.
5. To understand the process and techniques of spectroscopy.
6. To learn the advancement of spectroscopy.

7. To understand the various techniques with advantages, disadvantages/limitations and application of spectroscopy in industrial aspects.

Learning Outcome :

1. The students will understand the concept, importance and scope of UV-Visible spectroscopy.
2. Evaluate the utility of UV/Vis spectroscopy as a qualitative and quantitative method.
3. The students will understand the concept and importance of IR spectroscopy.
4. The students will understand the role of infrared spectroscopy in the study of structure of organic compounds
5. The student will understand the concept and application of NMR (^1H NMR and ^{13}C NMR) in organic synthesis as well as medicinal chemistry.
6. Students will learn fragmentation patterns by Mass spectroscopy.
7. To be able to analyze and interpret the spectral data collected from different spectroscopic techniques.
8. To be able to solve problems related to the structure, purity, and concentration of chemicals.
9. To gain valuable insight into the types of molecular interactions by choosing suitable spectroscopic methods and interpreting the obtained data.

Unit – I UV-Visible & IR Spectroscopy

UV-Visible Spectroscopy

Introduction, Principle, Selection rules for electronic transition, Electronic transitions, Solvent effects, Chromophore and auxochrome, Different shifts, Instrumentation, Applications, Problems based on dienes, enones, benzoyl derivatives

IR Spectroscopy

Introduction, Principle, Selection rule, Important group frequencies, Modes of vibration, Degree of freedom, Different peaks, Preparation method for samples, Instrumentation

Unit-II ^1H NMR and ^{13}C NMR

^1H NMR: Introduction, nuclear spin and magnetic nuclei, nuclear magnetic moment, behaviour of a bar magnet in a magnetic field, the

NMR transition measuring the chemical shift, shielding and de shielding of magnetic nucleus, chemical shifts in aliphatic and aromatic compounds, factors affecting chemical shift, Spin-spin splitting: effect of spin-spin splitting on the spectrum, mechanism of spin-spin splitting, chemical exchange, coupling constants (cis/trans, allylic system and aromatic ring); application of spin-spin splitting to structure determination-geminal-, vicinal-, long-range coupling; factors influencing geminal and vicinal coupling. simplification of the complex PMR spectra- (1) Increasing field strength (high resolution spectra), (2) Use of shift reagents, (3) Spin-spin decoupling (Double resonance), (4) Proton exchange, (5) Deuterium exchange, (6) Nuclear Over Hauser Effect (NOE) FT and two-dimensional NMR spectroscopy: principle of FT NMR- FIDs, Fourier transformation; ^1C , ^{13}C , ^{19}F , ^3P NMR-range of chemical shift values, spectra of typical examples; 2D NMR spectra- introduction and types of 2D techniques. 2D NMR Spectroscopy: Theory and Principles Of 2D NMR Spectroscopy (COSY); To interpret or to draw HOMCOR (^1H - ^1H COSY, DQFCOSY, INADEQUATE),

^{13}C NMR: Introduction, difficulties and solution for recording ^{13}C -NMR spectra; recording of ^{13}C -NMR spectra – scale, solvents, solvent signals and their positions, multiplicity, ^{13}C - ^1H coupling constant; proton coupled and decoupled ^{13}C spectra, broad band decoupling, off resonance technique; Chemical shifts in ^{13}C spectra – chemical shift calculation for alkanes, alkenes and alkynes, chemical shift calculation in internal and terminal substituted compounds, aromatic compounds; To identify structure from ^{13}C NMR data; Use of ^{13}C spectra in differentiating compounds/isomers; ^{13}C DEPT Spectra – Differentiation in Primary, Secondary and Tertiary Carbons by DEPT-45, DEPT-90, DEPT-135spectra. HETCOR (^{13}C - ^1H COSY, ^1H - ^{13}C COSY i.e. HMQC, HMBC), NOESY and TOCSY spectra.

Unit-III Mass spectrometry

Introduction, Determination of molecular weight and formulae, Parent peak, Base peak, Molecular ion peak, metastable peak, Ionization techniques (CI, FD, FAB, ESI, MALDI), Fundamental fragmentation process, Fragmentation patterns of organic functional groups, Examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

Unit-IV Problems/interpretation structure/structure determination based on UV, IR, ¹H NMR, ¹³C NMR, Mass spectrometry.

Spectral Problems Based on Combined Spectroscopy - DBE rules, Problems based on UV-Visible spectroscopy, Problems based on IR spectroscopy, Problems based on Mass spectrometry, Problems based NMR spectroscopy

Reference:

1. Spectrometric identification of organic compounds, T. C. Morrill, R. M. Silverstein and G. Bassler, 6th edition, John Wiley and sons.
2. Introduction to spectroscopy, D. L. Pavia, G. M. Lampman and G. S. Kriz, 3rd Ed., Harcourt college publishers.
3. Organic spectroscopy by W.Kemp.
4. Spectroscopic methods in organic chemistry, D. H. Williams and Ian Fleming
5. Organic spectroscopy by P.S. Kalsi

CHE(EO) 504 ELECTIVE-1

Medicinal & Industrial Chemistry

Learning objectives :

1. Students will about the medicinal and industrial chemistry.
2. Learns will get knowledge of Drug design.
3. Learns can understand how to synthesis various drugs.
4. Learns can understand how to purify various products at Research (R & D) labs and industrial scale.

Learning outcomes:

1. Drug design is the important task since the discovery of drug and in future drugs are the need of the society. Learns will understand the concepts of how to develop drug.
2. Learns will understand what are antibiotics and where/when to use them.
3. The chemist (learns) should know how to synthesis the drugs by best route of synthesis.

4. For any chemical products the raw materials are required. The learns will learn how to synthesize the raw materials by green chemistry aspects.
5. Learns will learn that how to isolate and purify the products at chemical industries.

Unit – I -Drug Design, Antibiotics and antimalarial (with SAR, MOA)

Drug Design

Introduction, naming of organic medicinal compounds, development of new drugs, procedure (conventional and recent/modern) followed in drug design, concept of lead compound and lead modification, pro drugs, soft drugs and hard drugs, phase I, II and III clinical trials, structure activity relationship, theories of drug activity : occupational theory, rate theory, induced fit theory, quantitative structure activity relationship. Concept of drug receptors, elementary treatment of drug receptor interactions, physio chemical parameters lipophilicity, partition coefficient, electronic ionization constant. Introduction to drug discovery by CADD - Structure and property, ADME-rules, concept of QSAR & 3-D QSAR, Pharmacophore, Enzymes/proteins structures/docking. Software used in drug design.

Antibiotics and antimalarial (with SAR and MOA)

Introduction, general classification, structural variations, synthesis and medicinal uses of the following :

Antibiotics: Penicillin, tetracycline, chloroamphenicol.

Antimalarial: Antimalarial agents based on 4-amino and 8-amino.

Unit –II –Organic synthesis of imp drugs (psychoactive, cardiovascular, hypoglycemic, anti-TB, antimalarial)

Psychoactive drugs

Thiopental, amobarbital, diazepam, chlorozepan, alprazolam, glutethimide, nikethamide, procaine, lidocaine and dibucaine, Ibuprofen, meclizine sodium, novalgine, pethidine

Cardiovascular, diuretics and hypoglycemic drugs

Synthesis of amyl nitrate, diltiazem, atenolol, methyl dopa, tolbutamide, chlorpropamide, glibenclamide, acetazolamide, chlorothiazide, furosemic and ethacrynic acid

Antimalarial drugs

Mefloquines, chloroquine, primaquine and daraprim

Antituberculosis drugs

Isoniazid (INH), Ethionamide, Ethambutol, DDS (Dapsone)

Unit – III- Basic principle and unit process (by Convention and Green chemistry aspects) in organic chemistry/industry

Basic principle at chemical industry

Basic chemical data (including MSDS), flow charts, chemical process selection, batch versus continuous operation. Safety – general safety, safety during handling of chemicals, fire safety. Hazardous - toxic chemical materials (Solid, liquid and gas), precaution and action taken during accident by chemicals. Patents and its importance in Research and development/chemical industry. Good manufacturing practice (GMP) and Good laboratory practice (GLP).

Unit process (in organic chemistry) at chemical industry

Nitration, Halogenation, Sulphonation and Amination methods and industrial chemicals derived from benzene, naphthalene using unit process by Convention and Green chemistry aspects (Green catalyst, Name reactions associated with green chemistry, one pot reaction, MCR, use of MW, Ultra sonic/sound) for each unit process with suitable examples.

Unit – IV - Separation (chromatography & Unit operations) Techniques and Applications in organic chemistry

Chromatography Techniques

TLC, HPTLC, GC, HPLC/LC, SFC, Column Chromatography, Combi Flash -...

Unit operations in organic chemistry –

Filtration – Different types of filtration techniques, filter aid and filter media.

Distillation - Different types of distillations with their pros and cons.

Extraction – Solid from solids and liquid from liquids using suitable reagents.

Drying – Using ovens, spray tower, plate and frame dryer

Reference:

1. Burger's medicinal chemistry and drug design (5/e) 1997, vol 1 to 5 edited by Manfred E. Woltt (John Wiley and Sons, New York)
2. Principles of medicinal chemistry by William A. Foye (1991), Lea and Febiger (Philadelphia)
3. Principles of medicinal chemistry vol I & II (5/e) F.S. Kadam, K.R. Mahadik and K.G. Bohra (Nirali publication)
4. Medicinal chemistry by Ashutosh Kar
5. The organic chemistry of drug synthesis vol I, II and III (1980) ed by D. Lednicher and L.A. Mitscher (John Wiley and Sons, New York)
6. Wilson and Gisvold text book of organic medicinal and pharmaceutical chemistry (5/e, 1982) by Robert Doerge (J.B. Lippincott Company, Philadelphia/ Toppan Co. Ltd, Tokyo)
7. Topics in medicinal chemistry vol I & II by Rabinowitz Myerson (Interscience 1968)
8. The pharmaceutical basis of therapeutics by Geoman and Gilman (McMillan Co.)
9. Unit processes in organic synthesis by P. H. Groggins
10. Industrial Chemical process by R. N. Shreve
11. Riegels handbook of industrial chemistry by James and Kent
12. Dryden's outlines of chemical Technology M. Gopal Rao

CHE(EO) 504 ELECTIVE-2

**ESSENTIALS OF OXIDATION, REDUCTION AND C-C BOND
FORMATION. APPLICATION IN ORGANIC SYNTHESIS**

<https://nptel.ac.in/courses/104/101/104101127/#>

COURSE PLAN:

Week 1: Introduction to organic synthesis, importance of selectivity and basics of oxidation of alcohols and development of sulfur based oxidations: Swern

oxidation and related concepts; Continuation of Swern oxidation and the utility of intermediates derived from Swern oxidation including Pummerer intermediates; Oxidations using selenium compounds such as SeO₂ and organoselenium compounds

Week 2: Dess-Martin, IBX and related hypervalent iodine based oxidations; Silver carbonate/celite, Prevost reactions and its modern variation. Microbial oxidations such as *Pseudomonas Putida* etc. Week 3: Oxidations with RuO₄ and other Transition metal catalysed oxidations; Tamao-Fleming Oxidation; Oxidations with Dimethyl dioxirane (DMDO) and 2-sulfonyloxaziridines and chiral versions; Oxidations at unfunctionalised carbons, Photosensitized oxidations

Week 4: Reduction of Carbonyl compounds with Boron and Aluminium based reagents such as Luche Reduction, NaCN(BH₃), DIBAL, Red-Al, L- and K-Selectrides, Superhydrides and associated selectivities.

Week 5: Low Valent Titanium species and Microbial reductions (NADH model etc.); Dissolving Metal Reductions; Reduction with Silanes

Week 6: Sharpless epoxidation and synthetic utility of the chiral epoxy alcohols; Katsuki-Jacobsen epoxidation and mechanistic details; OsO₄ based and related Sharpless Asymmetric Dihydroxylation

Week 7: Corey's oxazaborolidines in asymmetric reductions; Noyori's Ruthenium catalysed reduction of ketones; Asymmetric Hydrogenations with BINAP

Week 8: C-C Bond formation via Carbanions alpha to electron withdrawing groups; Boron and Silicon Enolates: Formation and Use in C-C Bond Formation; Imines in C-C Bond Formation; Simmons-Smith Cyclopropanation in Organic Synthesis

Week 9: Use of Allyl Boron, Allyl and Vinyl Silanes and Allyl Tin compounds in C-C Bond Formation

Week 10: Introduction to SAMP and RAMP chiral ligands for asymmetric C-C bond formation; Introduction to Oppolzers Sultam based chiral ligands and their reactions for organic synthesis; Evans Oxazolidinone for asymmetric synthesis

Week 11: Synthesis of selected natural products using above discussed methods of oxidation, reduction and C-C Bond formations

Week 12: Synthesis of selected natural products using above discussed methods of oxidation, reduction and C-C Bond formations

CHE(O) ELECTIVE-3

REAGENTS IN ORGANIC SYNTHESIS

<https://nptel.ac.in/courses/104/103/104103111/>

COURSE PLAN:

Week 1: Oxidizing Agents in Organic Transformations-Part-I

Week 2: Oxidizing Agents in Organic Transformations-Part-II

Week 3: Reducing Agents in Organic Transformations-Part-I

Week 4: Reducing Agents in Organic Transformations-Part-II

Week 5: Organic Transformations-Using Non-Transition Metals Part-I

Week 6: Organic Transformations-Using Non-Transition Metals Part-II

Week 7: Organic Transformations-Using Non-Transition Metals Part-III

Week 8: Organic Transformations-Using Transition Metals Part-I

Week 9: Organic Transformations-Using Transition Metals Part-II

Week 10: Organic Transformations-Using Transition Metals Part-III

Week 11: Organic Transformations-Using Transition Metals Part-IV

Week 12: Organic Transformations-Using Lanthanides Reagents

CHE(O) 505 PR & CHE(O) 506 PR

One or multi step preparation of Organic compounds and study of reaction, mechanism, mole ratio calculation, TLC, purification, confirmation by chemical method, UV, IR, Mass and NMR value of compound (Theoretical)

CHE(O) 505 PR

Product 35 (Reaction mechanism -10, Crude and crystal 20, Calculation & M.P./B.P - 5), Viva 15, TLC & Spectral data 20 = 70 Marks

Total marks 100 = 70 (External) + 30 (Internal)

1. p-Bromo benzene from Bromobenzene
2. Benzanilide from Benzoyl chloride & Aniline– Schotten Baumann Reaction
3. Hippuric acid from Benzoyl chloride & Glycine
4. Sulphanilic acid from Aniline
5. Sym-tribromobenzene from Aniline
6. m-Nitro phenol from m-Nitro aniline
7. Phenylazo-2-naphthol from aniline & 2-Naphthol
8. Diazobenzene from aniline
9. p-amino azabenzene - Diazobenzene & aniline
10. Hydrazobenzene from Nitrobenzene
11. Benzidine from Hydrazobenzene
12. p-Nitrophenylhydrazine from p-Nitroaniline
13. Cinnamic acid (Perkin reaction) from Benzaldehyde
14. Benzanilide from Benzophenone (Becmann reaction)
15. p-Benzoquinone – Hydroquinone

CHE(O) 506 PR

Product 35 (Reaction mechanism -10, Crude and crystal 20, Calculation & M.P./B.P - 5), Viva 15, TLC & Spectral data 20 = 70 Marks

Total marks 100 = 70 (External) + 30 (Internal)

1. Anthanilic acid from Phthalimide
2. Benzilic acid from benzoin (Benzilic acid rearrangement)
3. Benzimidazole/2-methyl benzimidazole from o-phenylene diamine
4. Adipic acid from Cyclohexanol
5. 4-Amino benzoic acid from 4-Nitro toluene
6. 4-Methyl-7-acetoxy coumarin from Resorcinol
7. p-Ethoxy acetanilide from p-Amino phenol
8. p-Bromoaniline from Acetanilide
9. Benzotriazole from o-phenylenediamine
10. p-Bromo aniline from aniline
11. Salicyldehyde from phenol
12. m-Nitro Phenol from m-nitro aniline
13. 8-nitro quinolone from o-nitro aniline
14. Congo red from Benzidine
15. Phenolphthalein from phenol

Reference:

1. *Small scale preparations by Arther I. Vogel*
2. *Practical Organic Chemistry, fourth edition by Mann & Saunders*
3. <http://orgsyn.org/> (*Organic syntheses*)

Sem. IV

CHE(O) 507 Scientific Writing

- ♦ Writing of Research Article/Review Article/Commentary Article/Case Study/Monograph/Book Chapter/Book Review/Research Proposal or any other scientific article type.
- ♦ The student can select any one scientific writing type or research proposal and submit a copy (hard and soft) of the same for internal and external evaluation.
- ♦ Evaluation shall be centered around on novelty, relevance, significance, and impact.
- ♦ Additional weightage will be given for submission/publishing of any article type in any journal (University journal or a journal that is indexed in the UGC CARE list/Web of Science/ SCOPUS/SCI/SCIE etc.) or a research proposal.

Guidelines for Scientific Writing

Research Article

Presents a full report with new results on a specific topic. Complete experimental details with proper justification. Generally not limited in length, with figures, tables, and references. Format...Title, Authors, Abstract, introduction, experimental, results, discussion, conclusion, acknowledgment, references

Review Articles/Commentary Article

Gives an overview of research in a particular field. It can be on one's own research or any other topic of general and current interest. Organized differently from communications or research articles as it does not have primary experimental data. Data of existing literature can be presented in a tabular format, graphs, diagrams, figures, charts etc. Should be referenced as thoroughly as possible. Format...Title, Authors, Abstract, introduction, discussion, conclusion, acknowledgment, references

Case Study

This study represents person, group, or situation that has been studied over time. Format depends upon the type of study.

Monograph

Title, Author, Introduction: Reason to select a topic; History, timeline, and Scientific/social significance; Benefits to the scientific community, teaching, and research, Development: Exposition of ideas into paragraphs or chapters. "Quote that authors endorse these ideas." Conclusion: Status and future perspectives, References: Should be referenced as thoroughly as possible

Book Chapter

Title, Authors, Abstract, Introduction/Background on the topic, Discussion (with subdivisions): Text with tables, figures, charts etc., Summary/Conclusion: Status and future perspectives, References

Book Review

A book review is a thorough description, critical analysis, and/or evaluation of the quality, meaning, and significance of a book, often written in relation to prior research on the topic.

Scope/Purpose/Content, Note the Method/Methodology of writing, Critically Evaluate the Contents, Examine the Front Matter and Back Matter, Summarize and Comment.

Research Proposal

Title, Research Problem/Problem Statement, Rational/Purpose of the Study
Review of the Literature, Proposed Research Framework, Research Questions/Proposed Hypothesis, Significance, Proposed Methods and Procedures, Deliverables/Expected Outcomes, Execution timelines, year wise breakup, Financial aspects, References

References

- 1 “*A Manual for Writers of Research Papers, Theses, and Dissertations*”, Kate Turabian, University of Chicago Press, 8th Edition, 2013.
- 2 “*Concise Guide to Writing Research Papers (Perfect Phrases Series)*”, Carol Ellison, McGraw-Hill Education; 1st Edition, 2010.

CHE(O) 508 Report Writing

- ♦ Report Writing for Participation and/or presentation (Poster/Oral/Invited talk as applicable) in University/State level/National/International Seminar/Conference/Webinar/ Symposium/Workshop/Hands-on training /Software learning of at least 2 days. In case of one day seminar/ webinar/ conference/workshop, it is mandatory to participate in two such events.
- ♦ Evaluation will be based on detailed technical report prepared on the conference/seminar/workshop participated and for Poster/Oral presentation, as applicable.
- ♦ Additional weightage will be given for Poster/Oral presentations.

Guidelines for Report Writing

It aims to summarise the most important talks/research presented. It is not usually feasible to attempt comprehensive coverage of the conference. More focus should be on those presentations that are most topical, interesting, or thought-provoking.

Points to consider when writing the report:

- Name of Institute/Department/University that organized the conference
- Title and theme of the conference
- Information regarding number of attendees, where and when it was held (date), name of the convener, organizing secretary etc.
- Include a copy of the brochure
- A brief about the Inaugural Session
- Details of all the technical sessions
- List of main speakers, their position/designation, topic, expertise, and their institutional affiliation
- Highlight research paper(s) or work with major significance and impact
- A brief about the Concluding/Valedictory Session
- Embed the text with photographs wherever possible
- The outcome/summary: Your learning

References

- 1 “*Writing for Conferences: A Handbook for Graduate Students and Faculty*”, Leo Mallette, Clare Berger, Greenwood; Illustrated Edition, 2011.
- 2 “*The Creative Writing Handbook*”, John Singleton (Editor), Mary Luckhurst (Editor), Red Globe Press; 2nd Edition, 1999.

CHE(O) 509 Industrial Training/ NET-GSET based Test

Guidelines for Industrial Training

- 1 Each student must undergo 3 weeks industrial training under the supervision of a faculty from the concerned department.
- 2 The industry may be in Ahmedabad, Gujarat or anywhere in India.
- 3 The training may be obtained at any R&D, QA, QC, Production or any other relevant department on different instrumental techniques or other laboratory equipments.

- 4 The students must submit a report on the training obtained from the industry which may include (a) introduction about the industry (b) various activities of the industry (c) the process which are used in the industry (d) the products of the industry and (e) summary and conclusion.
- 5 The report submitted by each student would be assessed by the branch in-charge and the supervising teacher.
- 6 The student must discuss/present the details of the training through a power point presentation

NET-GSET based Test

50% from Sem. I & II, 50% from Sem. III syllabus but the question/exam pattern will be based on CSIR-NET or GSET.

CHE(O) 510 Dissertation

Guidelines for Dissertation/Project Work

- 1 Each student must carry out a project under the supervision of a faculty from the concerned department.
- 2 The project can be carried out either in the department or in any other industry, institute or organizations located in Ahmedabad, Gujarat or anywhere in India.
- 3 The topics of the dissertation can be selected from any of the four branches of chemistry i.e., Organic, Inorganic, Physical or Analytical. The topic can be related to (a) synthesis, purification, characterization, application of organic compounds or (b) metal complexes preparation and applications or (c) physical studies of various systems (d) method development and validation (e) green chemistry (f) nanomaterials preparation and applications (g) functionalized supramolecules (h) electro analytical methods (i) environmental analysis and decontamination or any other related to the subject.
- 4 Each student must submit a dissertation on the topic of their study comprising of (a) an introduction on the topic along with literature survey and justification for the selection of the topic (b) materials and methods (c) methodology (d) results and discussion and (e) summary and conclusion along with the references.
- 5 Each student must give monthly report and a midterm presentation of their work at the department.
- 6 The student must discuss/present the details of dissertation through a power point presentation.
- 7 Dissertation would be examined by the supervising teacher and external examiner.

GUJARAT UNIVERSITY
MSc Physical Chemistry Semester III and IV
Revised Syllabus
Design and Structure of Choice Based Credit System
(Effective from 2021-2022)

| MSc Semester III | | | | | | |
|-------------------------|---------------------------------------|--|-------------------|-----------|---------------|------------|
| Course | | No. of hours per week (12 h for each unit and 48 h for each paper/course) | | | Total credits | Marks |
| Paper Code | Type | Lectures | Labs | Total | | |
| CHE (P) 501 | Core Paper | 4 | -- | 4 | 4 | 100 |
| CHE (P) 502 | Core Paper | 4 | -- | 4 | 4 | 100 |
| CHE (P) 503 | Core Paper | 4 | -- | 4 | 4 | 100 |
| CHE (EP) 504 | Elective Paper | 4 | -- | 4 | 4 | 100 |
| CHE (P) 505 PR | Lab Course 1 | -- | 6 | 6 | 4 | 100 |
| CHE (P) 506 PR | Lab Course 2 | -- | 6 | 6 | 4 | 100 |
| | Total | 16 | 12 | 28 | 24 | 600 |
| MSc Semester IV | | | | | | |
| Course | | No. of hours per week (12 h for each unit and 48 h for each paper/course) | | | Total credits | Marks |
| Paper Code | Type | Lectures/ Discussion | DISS/PW and IT | Total | | |
| CHE (P) 507 | Core Paper (Scientific Writing) | 4 | -- | 4 | 4 | 100 |
| CHE (P) 508 | Core Paper (Report Writing) | 4 | -- | 4 | 4 | 100 |
| CHE (P) 509 | Core paper (Industrial Training, IT) | -- | 5 | 5 | 4 | 100 |
| CHE (P) 510 | Dissertation (DISS)/Project Work (PW) | -- | 15 | 15 | 12 | 300 |
| | | 08 | 20 | 28 | 24 | 600 |

For each paper 30 % weightage is given to internal assessment and 70 % for external assessment.

M. Sc Semester-III
CHE(P) 501 Advanced Physical Chemistry

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| | Learning Objectives: |
| 1. | To describe the assumptions made in the Kinetic theory of gases, To describe how the distribution of speed of gases change with temperature, To understand the significance of Kinetic molecular theory of gases which describe the behavior of gases. |
| 2. | To brief about principle of FTIR spectroscopy, to explain about the fundamentals of the bonds. |
| 3. | To explain about classical and quantum theories of Raman spectroscopy, applications of Raman Spectroscopy. |
| 4. | To brief about the different properties of solid. To discuss about the liquid crystals. |
| | Learning Outcomes: |
| | After the end of the course student will be able to |
| 1. | Calculate the distribution of speeds, explain the behavior of gases. |
| 2. | Interpret FTIR spectroscopy, Explain the working principle and taking spectrum of IR spectroscopy device. |
| 3. | To understand the basic principle of Raman spectroscopy and its various applications. |
| 4. | Use the properties the solids |

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| Unit-I | Gaseous state of matter: Introduction, Barometric distribution law, Maxwell's law of distribution of molecular velocities, effects of temperature and significance, Maxwell distribution as energy distribution, Types of molecular velocities: Average, root mean square and most probable velocities, equipartition of energy and quantization, The kinetic gas equation, Kinetic energy and temperature. |
| Unit-II | IR and FT-IR spectroscopy: Introduction, Vibration in diatomic molecules, Harmonic oscillations in diatomic molecules, Anharmonic Oscillations in diatomic molecules, Selection rules, Force constant, Bond strength and bond length, Simultaneous vibration and rotational transitions, FT-IR : Principles and techniques. |
| Unit-III | Raman Spectroscopy: Introduction, Light scattering by molecules, Classical and quantum theory of Raman effects, Pure rotational, Pure vibrational and vibrational and rotational Raman spectra and selection rules, general mechanism of Raman effect, Raman effects in liquids, gases and solids, Applications of Raman effect in Physical Chemistry. |

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| Unit-IV | <p>The solid state: Introduction, Mechanical properties of solids: Electrical properties of solids: conductors, Insulators and semiconductor, super conductors, Band theory of solids, insulators and semiconductors, super conductors, BCS theory of super conductors, Magnetic properties of solids, liquid crystals and its applications. Ferro magnetism and anti ferromagnetism, measurements of magnetic susceptibilities.</p> |
|----------------|--|

References:

1. Introduction to Physical Chemistry-Glasstone
2. Physical Chemistry-Atkins
3. Advanced Physical Chemistry-Gurdeep Raj: Goel publishing House
4. Comprehensive Physical Chemistry-N. B. Singh, N. S. Gajbhiye, Shiva Saran Das: New Age International Publication
5. Advanced Physical Chemistry-J. N. Gurtu and A. Gurtu, Pragati prakashan
6. Wiley Engineering Chemistry Second Edition
7. Molecular Spectroscopy-C. N. Banwell and E. M. McCash: Mc Graw Hill Education
8. Introduction to Molecular Spectroscopy-G. M. Barrow: Mc Graw Hill Education
9. Physical Chemistry for the Chemical and Biological Sciences-Raymond Chang: University Science Books
10. Handbook of Instrumental Techniques for Analytical Chemistry-Frank A. Settle, Editor: Pearson Education
11. Basic Principles of Spectroscopy-R. Chang McGraw Hill
12. Instrumental methods of Analysis-Skoog and West
13. Instrumental Methods of Chemical Analysis-B. K. Sharma: Krishna Prakashan Media(P) Ltd. Meerut
14. Physical Methods of Chemistry-R. S. Drago
15. Principles of Solid State-H. V. Keer
16. Solid State Chemistry-N. B. Hannay
17. Solid State Chemistry-C. N. R. Rao
18. Solid State Chemistry-R. C. Ropp: Elsevier
19. Principles of Physical Chemistry-Puri, Sharma and Pathania: Vishal Publishing Co.
20. Textbook of Physical Chemistry-p. L. Soni, O. P. Dharmarha and U. N. Dash: Sultan Chand and Sons
21. Physical Chemistry-Dr. S. Parari: New Central Book Agency (p) Ltd.

M. Sc Semester-III
CHE(P) 502 Selected topics in Physical Chemistry

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| | Learning Objectives: |
| 1. | To discuss about the exchange of mass, energy in the gaseous system, to discuss about the collision parameters. |
| 2. | To brief about the different properties of solid. |
| 3. | To discuss about the basic principle of absorption, application of the principle, |
| 4. | To discuss about the laws of photochemistry, to discuss about the earth atmosphere, |
| | Learning Outcomes: Upon completion of the course student will be able to |
| 1. | Understand the mass and energy transfer of the gases, able to calculate the molecular parameters, mean free path, collision frequency. |
| 2. | Determine the structure of Crystalline materials, determine the particle size. The crystal size distribution in study the reaction rate. |
| 3. | Can explain the origin of UV visible absorption spectra, detect environmental contamination. |
| 4. | To form some typical compounds and cleaning agents. |

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| Unit-I | Transport phenomenon in gases: Introduction, Transport properties: Thermal conductivity, viscosity and diffusion, Collision parameters: collision diameter, collision cross section, collision number, collision frequency, mean free path, van der Waals equation of state for real gases, Graham's law of effusion and diffusion. |
| Unit-II | Diffraction techniques: Introduction, The Bragg's equation, Structural determination by X-rays: Powder method, Laue method, Debye-Scherrer method, Indexing and determination of lattice parameters of a unit cell of NaCl, Graphical method of indexing, Rietveld analysis, determination of particle size of crystallites. |
| Unit-III | Visible and electronic spectroscopy: Introduction, Lambert-Beer's law, regression and correlation coefficient, Ringbom plot, Applications: analysis of mixtures, determination of Pka, electronic spectra of diatomic molecules, Franck-Condon principle, Concept of potential energy curves for bonding and antibonding molecular orbitals, selection rules, molecular orbitals their energy levels, and respective transitions. |
| Unit-IV | Photochemistry: |

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| Introduction, Laws of photochemistry: First law, second law stark Einstein law of photochemical equivalence, quantum efficiency, low and high quantum yield, experimental method for the determination of quantum yields, action spectrum, Earth's atmosphere: composition of the atmosphere, region of the atmosphere, Residence time, The Greenhouse effect, photochemical smog, formation of nitrogen oxide, formation of O ₃ , secondary pollutants, harmful effects and prevention of photochemical smog. |
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References:

1. Introduction to Physical Chemistry-Glasstone
2. Physical Chemistry-Atkins
3. Advanced Physical Chemistry-Gurdeep Raj: Goel publishing House
4. Comprehensive Physical Chemistry-N. B. Singh, N. S. Gajbhiye, Shiva Saran Das: New Age International Publication
5. Advanced Physical Chemistry-J. N. Gurtu and A. Gurtu, Pragati prakashan
6. Wiley Engineering Chemistry Second Edition
7. Molecular Spectroscopy-C. N. Banwell and E. M. McCash: Mc Graw Hill Education
8. Introduction to Molecular Spectroscopy-G. M. Barrow: Mc Graw Hill Education
9. Physical Chemistry for the Chemical and Biological Sciences-Raymond Chang: University Science Books
10. Handbook of Instrumental Techniques for Analytical Chemistry-Frank A. Settle, Editor: Pearson Education
11. Basic Principles of Spectroscopy-R. Chang McGraw Hill
12. Instrumental methods of Analysis-Skoog and West
13. Instrumental Methods of Chemical Analysis-B. K. Sharma: Krishna Prakashan Media(P) Ltd. Meerut
14. Physical Methods of Chemistry-R. S. Drago
15. Principles of Solid State-H. V. Keer
16. Solid State Chemistry-N. B. Hannay
17. Solid State Chemistry-C. N. R. Rao
18. Solid State Chemistry-R. C. Ropp: Elsevier
19. Principles of Physical Chemistry-Puri, Sharma and Pathania: Vishal Publishing Co.
20. Textbook of Physical Chemistry-p. L. Soni, O. P. Dharmarha and U. N. Dash: Sultan Chand and Sons
21. Physical Chemistry-Dr. S. Parari: New Central Book Agency (p) Ltd.

M. Sc Semester-III
CHE(P) 503 Polymer Chemistry

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| | Learning Objectives: |
| 1. | The objectives of the course are to explain about concept of molecular weight, methods of determining molecular weight, to explain about the concept of molecular weight distribution, |
| 2. | To describe about the molecular structures and its significance, effect of temperature of properties of polymers. |
| 3. | To describe the effect of size and shape of polymers on its properties |
| 4. | To describe about thermodynamics and processing of Polymers and its application. |
| | Learning Outcomes: |
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| 1. | To synthesize polymers and to determine the molecular weight by different methods, |
| 2. | To process polymers by different processes, |
| 3. | The knowledge of polymers helps to use in different fields. |
| 4. | Change the properties by applying the principle of thermodynamics and characterize polymers. |

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| Unit-I | Polymer molecular weight and characterization: Introduction, concepts of molecular weight distribution, Measurements of molecular weight and size: Viscosity, light scattering, osmometry and ultracentrifuge methods, Molecular weight and degree of polymerization, polydispersity and molecular weight distribution in polymers, The practical significance of Polymer molecular weight, size of polymer molecules. |
| Unit-II | Structure and properties of polymers: Introduction, polymer microstructure, microstructures based on the chemical and geometrical structure, Crystalline structure of polymers, Glass transition temperature (T _g) and molecular weight, Glass transition temperature and melting point, importance of glass transition temperature, The mechanical properties of crystalline polymers, Properties involving large deformation: Melting point, tensile strength and related properties. |
| Unit-III | Polymer processing: Plastic technology: compression molding, injection molding, blow molding, rotational molding and thermoset molding, Extrusion, coextrusion, film extrusion, |

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| | pultrusion, calendering, casting. Fiber technology: Textile and fabric properties, spinning, fiber after treatments. |
| Unit-IV | Polymer solutions: Introduction, the process of polymer dissolution, Thermodynamic of polymer solution, The Flory-Huggins theory of polymer solution, nature of polymer molecules in solution, Size and shape of macromolecules in solution, viscosity of diluted and concentrated polymer solution. |

References:

1. Polymer chemistry - Flory
2. Polymer science - Hiemenz
3. Text Book of Polymer Science - Fred W. Billmeyer: Wiley
4. Principles of Polymer Science - P. Bahadur and N. V. Sastry: Narosa Publishing House
5. Polymer Science - V. R. Gowariker, N. V. Viswanathan and Jayadev Sreedhar: New Age International Publisher
6. Wiley Engineering Chemistry Second Edition
7. Specialty polymers – R. W. Dyson
8. Polymer characterization -E. Shroder, Hanser publication
9. Polymer process engineering – R. G. Dyson
10. Physical Chemistry of polymers – A. Tager, Mir publication, Moscow
11. Polymer chemistry – B. K. Sharma, Krishna prakashan, Meeraut

M. Sc Semester-III
CHE(EP) 504 Elective Paper-I (Special topics in Physical Chemistry)

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| | Learning Objectives: |
| 1. | To explain about enzymes and how it binds to an active site in the substrate and feasibility of reaction and reaction rate. |
| 2. | To focuses on importance of enzymes in biological processes and their functions and the effects of different factors. |
| 3. | To explain the classification of nano materials, types and their synthesis. |
| 4. | To describe various techniques to determine the structure. |
| | Learning Outcomes: |
| 1. | The student can able to describe and explain the basic principles of enzyme catalytic process. |
| 2. | Student can able to describe and explain the chemistry of oxygen binding to hemoglobin and myoglobin |
| 3. | Able to classify nano materials, can able to synthesis nano particles |
| 4. | Can able to understand the principles of instrumental techniques and determine the structures, properties and uses. |

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| Unit-I | Enzyme catalysis: Introduction, General principles of catalysis, Phase transfer catalysis, the equation of enzyme kinetics, Michaelis-Menten kinetics, steady-state kinetics, significance of K_M and V_{max} , Allosteric Interactions: Oxygen binding to Myoglobin and Hemoglobin, The Hill equation, Conformational Changes in Hemoglobin induced by Oxygen binding. |
| Unit-II | Enzyme Applications: Enzyme applications in Pharmaceuticals, The food-water-fuel nexus, Natural gas Conversation, food and Beverage industries, Flavors, Aromas and detergent industries. |
| Unit-III | Nano materials-I: Introduction, Classification of nano materials, Synthesis, Synthesis of Gold nano particles, Different types of nano structures: nanoparticles, nanowires, nanorods, nanotubes, nanofilms, C-nanotubes and nanoclusters. Advantages of nanoparticles, |
| Unit-IV | Nano materials-II: Introduction, Characterization: Scanning electron microscopy (SEM), Transmission electron microscopy (SEM), Scanning Tunneling microscopy, Atomic force microscopy (AFM), X-ray diffraction, Fluorescence spectroscopy. Applications. |

References:

1. Advanced Physical Chemistry-Gurdeep Raj: Goel publishing House
2. Comprehensive Physical Chemistry-N. B. Singh, N. S. Gajbhiye, Shiva Saran Das: New Age International Publication
3. Wiley Engineering Chemistry Second Edition
4. Principles of Physical Chemistry-Puri, Sharma and Pathania: Vishal Publishing Co.
5. Textbook of Physical Chemistry-P. L. Soni, O. P. Dharmarha and U. N. Dash: Sultan Chand and Sons
6. Physical Chemistry-Dr. S. Parari: New Central Book Agency (p) Ltd.
7. Nanoparticles – Mechanics and Mechanisms – K. T. Ramesh
8. L. Foster, Nanotechnology: Science, Innovation and opportunity, prentice Hall.
9. G. Cao, Nanostructures and Nanomaterials: Synthesis, Properties and Applications – Imperial College Press, London, 2004

M. Sc Semester-III
CHE(EP) 504 Elective Paper-II Polymer Chemistry

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| | Learning Objectives: |
| 1. | To discuss about characterization of polymers, solubility of polymers and the thermodynamics and related thermal properties |
| 2. | To brief about various processing techniques and the properties associated with various forms of polymers |
| 3. | To discuss about various reactions and its uses to prepare polymers with specific properties |
| 4. | To explain the various techniques to analyze and testing of polymers |
| | Learning Outcomes: |
| 1. | Student will be able to characterize polymers and be able testing various properties |
| 2. | Can be able to understand various processing techniques and its various applications |
| 3. | Student can be able to prepare various polymers with different properties using various reaction mechanisms |
| 4. | Be able to understand the various instrumental techniques and be able to analyze and testing of various polymers |

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| Unit-I | Characterization of Polymers: Introduction, Polymer solution: Criteria of polymer solubility, Conformations of dissolved polymer chain, Thermodynamics of polymer solutions, Solution viscosity and molecular size, Physical testing:- Mechanical properties: Stress-strain properties in tension, Impact tests, Hardness, Thermal properties: Softening temperature, Chemical properties: Resistance to solvent, Weathering. |
| Unit-II | Polymer Processing; Introduction, Plastic technology:- Molding: Compression molding, Injection molding, Blow molding, Rotational molding, Extrusion, Calendaring, Coating, Foaming, Fiber technology: Fiber properties and spinning. |
| Unit-III | Polymer Reactions: Introduction, Hydrolysis, Aminolysis, Hydrogenation, Reaction of Various specific groups: hydroxyl group, Aldehyde group, Ketonic and carboxylic groups, Cross-linking reactions, Block and Graft copolymers: Grafting by means of free radicals and through functional groups, |
| Unit-IV | Analysis and Testing of Polymers: Analysis of Polymers by Infrared Spectroscopy, NMR Spectroscopy, X-Ray diffraction, Microscopy: Electron microscopy, Scanning electron microscopy, |

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| Thermal Analysis and Applications: Thermogravimetric analysis, Differential thermal analysis, Differential scanning Calorimetry. |
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References:

1. Polymer chemistry - Flory
2. Polymer science - Hiemenz
3. Text Book of Polymer Science - Fred W. Billmeyer: Wiley
4. Principles of Polymer Science - P. Bahadur and N. V. Sastry: Narosa Publishing House
5. Polymer Science - V. R. Gowariker, N. V. Viswanathan and Jayadev Sreedhar: New Age International Publisher
6. Wiley Engineering Chemistry Second Edition
7. Specialty polymers – R. W. Dyson
8. Polymer characterization -E. Shroder, Hanser publication
9. Polymer process engineering – R. G. Dyson
10. Physical Chemistry of polymers – A. Tager, Mir publication, Moscow
11. Polymer chemistry – B. K. Sharma, Krishna prakashan, Meeraut

M. Sc Semester-III
CHE(EP) 504 Elective Paper-III Catalysis

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| | Learning Objectives: |
| 1. | To discuss briefly about classification of catalytic process, theory related to catalytic processes characterization and its applications |
| 2. | To brief about homogeneous catalysis, the method of its preparation and its applications |
| 3. | To discuss about the principle of PTC, advantages, structures and related properties of crown ethers |
| 4. | To brief about some industrial PT processes and its application |
| | Learning Outcomes: |
| 1. | Student can be able to classify, compare and can understand the general features of various catalytic processes |
| 2. | Student can be able prepare catalysts and understand the characterization techniques |
| 3. | Student can able to classify, understand the basic principles PTC and can able to carry out various reactions based on the structures |
| 4. | Student can be able to carry out various reactions of PTC and be able to apply in the manufacturing of various industrial products |

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| Unit-I | Homogeneous Catalysis: Introduction, Classification of Catalysis, General Features of catalysts, Comparison between Homogeneous and Heterogeneous Catalysis, General Features of Catalysts, Intermediate compound formation theory of Homogeneous catalysis and its Limitations, Characterization of Catalysts, Selectivity, Effective Atomic Number Rule (EAN), Some Industrial Applications of Catalysts. |
| Unit-II | Heterogeneous Catalysis: Introduction, Methods of Preparation of Catalysts, Characterization Techniques, Adsorption Theory of Heterogeneous Catalysis, Kinetics of Heterogeneous Catalysis, Effect of Temperature on Heterogeneous Reactions, Classification of Catalysis, Heterogeneous Catalytic Process used at Industrial Scale. |
| Unit-III | Phase Transfer Catalysis: Introduction, Types of Phase Transfer Catalysts, Principle of Phase Transfer catalysis, Mechanisms of Phase transfer Catalysis, Advantages of Phase Transfer Catalysts, Quaternary ammonium and phosphonium salts, crown ethers, their structures and properties. |
| Unit-IV | Industrial Phase transfer Catalytic Processes: |

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| Introduction, Oxidation, Alkylation, Hydrogenation, Dehydrohalogenation, Cynation, Aldol condensation, Some Heterogeneous catalytic processes used at industrial scale, Industrial Applications of Phase Transfer Catalysts. |
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References:

1. Advanced Physical Chemistry-Gurdeep Raj: Goel publishing House
2. Comprehensive Physical Chemistry-N. B. Singh, N. S. Gajbhiye, Shiva Saran Das: New Age International Publication
3. Wiley Engineering Chemistry Second Edition
4. Principles of Physical Chemistry-Puri, Sharma and Pathania: Vishal Publishing Co.
5. Textbook of Physical Chemistry-P. L. Soni, O. P. Dharmarha and U. N. Dash: Sultan Chand and Sons
6. Physical Chemistry-Dr. S. Parari: New Central Book Agency (p) Ltd.
7. Nanoparticles – Mechanics and Mechanisms – K. T. Ramesh
8. L. Foster, Nanotechnology: Science, Innovation and opportunity, prentice Hall.
9. G. Cao, Nanostructures and Nanomaterials: Synthesis, Properties and Applications – Imperial College Press, London, 2004

M. Sc Semester-III

CHE(P) 505 and 506 PR Physical Chemistry Practical

Thermodynamics:

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| 1. | To determine the Ultrasonic velocity and hence the acoustical parameters of water, Benzene and Cyclohexane. |
| 2. | To determine the adiabatic/isentropic Compressibility Ks of Benzene in Water and cyclohexane in Water. |
| 3. | To determination of thermodynamic parameters, effects of concentration, nature of solvent and solute on acoustical parameters. |

Spectrophotometry:

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|----|---|
| 1. | To determine the indicator constant of Phenolphthalein indicator. |
| 2. | To determine the composition of a binary mixture containing KMnO_4 and $\text{K}_2\text{Cr}_2\text{O}_7$. |
| 3. | To determine the composition and stability constant of a complex formed between Fe^{III} ions and Salicylic acid by Job's method of continuous variation. |
| 4. | To determine the adsorption of methylene blue on charcoal. |
| 5. | To determine the partial molar volume and the excess volume of the binary mixture of ethanol and water. |
| 6. | To determine the glass transition and melting temperature of polymer by DTA technique. |

Conductometry:

| | |
|----|---|
| 1. | To determine the stability constant of a complex and to evaluate the thermodynamic parameters and to check the effect of solvent and its composition on the stability of the complex. |
| 2. | To determine the hydrolysis constant of aniline hydrochloride by conductometry method. |
| | To determine the kinetic parameters V_{max} and K_m for catalysis of starch by enzyme alpha amylase. |

Chemical Kinetics:

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|----|--|
| 1. | To study the autocatalytic reaction between KMnO_4 and $\text{K}_2\text{Cr}_2\text{O}_7$. |
| 2. | To study the reaction between acetone and Iodine. |
| 3. | To determine the critical micelles concentration of sodium Laurel sulphate from the measurement of conductivity at different concentrations. |
| 4. | To find the stability constant of Ag- NH_3 complex. |

Reference books:

| | |
|----|--|
| 1. | Practical's in "Physical Chemistry" a Modern Approach P S Sindhu: Macmillan India Ltd. ISBN 1403 929165 |
| 2. | Experiments in Chemistry D. V. Jahagirdar: Himalaya Publishing House ISBN 81-7866-679-0 |
| 3. | Experimental Physical Chemistry R C Das, B Behera: Tata McGraw-Hill Publishing Company Limited, ISBN 0-07-451571-3 |
| 4. | Experimental Physical Chemistry V. D. Athawale, Parul Mathur: New Age International Publishers, ISBN 81-224-1336-6 |
| 5. | Experiments in Physical Chemistry (Instrumental and Physico-Chemical) Dr. P. H. Parsania, Dr. Falguni Karia |
| 6. | Advanced Practical Physical Chemistry J. B. Yadav: Krishna Prakashan Media(P) Ltd., Meerut ISBN 81-8283-916-5 |
| 7. | Experiments in Chemistry D. V. Jahagirdar: Himalaya Publishing House ISBN 81-7866-679-0 |

SEMESTER – IV (Physical Chemistry)

CHE(P) 507 Scientific Writing

- ♦ Writing of Research Article/Review Article/Commentary Article/Case Study/Monograph/Book Chapter/Book Review/Research Proposal or any other scientific article type.
- ♦ The student can select any one scientific writing type or research proposal and submit a copy (hard and soft) of the same for internal and external evaluation.
- ♦ Evaluation shall be centered around on novelty, relevance, significance, and impact.
- ♦ Additional weightage will be given for submission/publishing of any article type in any journal (University journal or a journal that is indexed in the UGC CARE list/Web of Science/ SCOPUS/SCI/SCIE etc.) or a research proposal.

Guidelines for Scientific Writing

Research Article

Presents a full report with new results on a specific topic. Complete experimental details with proper justification. Generally not limited in length, with figures, tables, and references. Format...Title, Authors, Abstract, introduction, experimental, results, discussion, conclusion, acknowledgment, references

Review Articles/Commentary Article

Gives an overview of research in a particular field. It can be on one's own research or any other topic of general and current interest. Organized differently from communications or research articles as it does not have primary experimental data.

Data of existing literature can be presented in a tabular format, graphs, diagrams, figures, charts etc. Should be referenced as thoroughly as possible. Format...Title, Authors, Abstract, introduction, discussion, conclusion, acknowledgment, references

Case Study

This study represents person, group, or situation that has been studied over time. Format depends upon the type of study.

Monograph

Title, Author, Introduction: Reason to select a topic; History, timeline, and Scientific/social significance; Benefits to the scientific community, teaching, and research, Development: Exposition of ideas into paragraphs or chapters.

“Quote that authors endorse these ideas.” Conclusion: Status and future perspectives, References: Should be referenced as thoroughly as possible

Book Chapter

Title, Authors, Abstract, Introduction/Background on the topic, Discussion (with subdivisions): Text with tables, figures, charts etc., Summary/Conclusion: Status and future perspectives, References

Book Review

A book review is a thorough description, critical analysis, and/or evaluation of the quality, meaning, and significance of a book, often written in relation to prior research on the topic. Scope/Purpose/Content, Note the Method/Methodology of writing, Critically Evaluate the Contents, Examine the Front Matter and Back Matter, Summarize and Comment.

Research Proposal

Title, Research Problem/Problem Statement, Rational/Purpose of the Study, Review of the Literature, Proposed Research Framework, Research Questions/Proposed Hypothesis, Significance, Proposed Methods and Procedures, Deliverables/Expected Outcomes, Execution timelines, year wise breakup, Financial aspects, References

References

- 1 “*A Manual for Writers of Research Papers, Theses, and Dissertations*”, Kate Turabian, University of Chicago Press, 8th Edition, 2013.
- 2 “*Concise Guide to Writing Research Papers (Perfect Phrases Series)*”, Carol Ellison, McGraw-Hill Education; 1st Edition, 2010.

SEMESTER – IV (Physical Chemistry)

CHE(P) 508 Report Writing

- ◆ Report Writing for Participation and/or presentation (Poster/Oral/Invited talk as applicable) in University/State level/National/International Seminar/Conference/Webinar/ Symposium/Workshop/Hands-on training/Software learning of at least 2 days. In case of one day seminar/ webinar/ conference/workshop, it is mandatory to participate in two such events.
- ◆ Evaluation will be based on detailed technical report prepared on the conference/seminar/workshop participated and for Poster/Oral presentation, as applicable.
- ◆ Additional weightage will be given for Poster/Oral presentations.

Guidelines for Report Writing

It aims to summarise the most important talks/research presented. It is not usually feasible to attempt comprehensive coverage of the conference. More focus should be on those presentations that are most topical, interesting, or thought-provoking.

Points to consider when writing the report:

- Name of Institute/Department/University that organized the conference
- Title and theme of the conference
- Information regarding number of attendees, where and when it was held (date), name of the convener, organizing secretary etc.
- Include a copy of the brochure
- A brief about the Inaugural Session
- Details of all the technical sessions
- List of main speakers, their position/designation, topic, expertise, and their institutional affiliation
- Highlight research paper(s) or work with major significance and impact
- A brief about the Concluding/Valedictory Session
- Embed the text with photographs wherever possible
- The outcome/summary: Your learning

References

- 1 “*Writing for Conferences: A Handbook for Graduate Students and Faculty*”, Leo Mallette, Clare Berger, Greenwood; Illustrated Edition, 2011.
- 2 “*The Creative Writing Handbook*”, John Singleton (Editor), Mary Luckhurst (Editor), Red Globe Press; 2nd Edition, 1999.

SEMESTER – IV (Physical Chemistry)

CHE(P) 509 Industrial Training

Guidelines for Industrial Training

- 1 Each student must undergo 3 weeks industrial training under the supervision of a faculty from the concerned department.
- 2 The industry may be in Ahmedabad, Gujarat or anywhere in India.
- 3 The training may be obtained at any R&D, QA, QC, Production or any other relevant department on different instrumental techniques or other laboratory equipments.
- 4 The students must submit a report on the training obtained from the industry which may include (a) introduction about the industry (b) various activities of the industry (c) the process which are used in the industry (d) the products of the industry and (e) summary and conclusion.
- 5 The report submitted by each student would be assessed by the branch in-charge and the supervising teacher.
- 6 The student must discuss/present the details of the training through a power point presentation

SEMESTER – IV (Physical Chemistry)

CHE(P) 510 Dissertation

Guidelines for Dissertation/Project Work

- 1 Each student must carry out a project under the supervision of a faculty from the concerned department.
- 2 The project can be carried out either in the department or in any other industry, institute or organizations located in Ahmedabad, Gujarat or anywhere in India.
- 3 The topics of the dissertation can be selected from any of the four branches of chemistry i.e., Organic, Inorganic, Physical or Analytical. The topic can be related to (a) synthesis, purification, characterization, application of organic compounds or (b) metal complexes preparation and applications or (c) physical studies of various systems (d) method development and validation (e) green chemistry (f) nanomaterials preparation and applications (g) functionalized supramolecules (h) electro analytical methods (i) environmental analysis and decontamination or any other related to the subject.
- 4 Each student must submit a dissertation on the topic of their study comprising of (a) an introduction on the topic along with literature survey and justification for the selection of the topic (b) materials and methods (c) methodology (d) results and discussion and (e) summary and conclusion along with the references.
- 5 Each student must give monthly report and a midterm presentation of their work at the department.
- 6 The student must discuss/present the details of dissertation through a power-point presentation.
- 7 Dissertation would be examined by the supervising teacher and external examiner.