

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

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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 NH_4Cl in a given mixture.



Potentiometry

1. To determine the standard redox potential and the number of electrons involved in $\text{Fe}^{+2}/\text{Fe}^{+3}$ 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 Na_2CO_3 and NaHCO_3 in the given mixture.



Chemical Kinetics and Adsorption

1. To study the effect of ionic strength of ions on the kinetics of the reaction $\text{S}_2\text{O}_8^{-2} + 2\text{I}^- \longrightarrow 2\text{SO}_4^{-2} + \text{I}_2$
2. To determine the temperature coefficient and energy of activation of reaction between $\text{K}_2\text{S}_2\text{O}_8 + \text{KI}$.
3. To determine the order of reaction between $\text{K}_2\text{S}_2\text{O}_8 + \text{KI}$ 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 Czako, 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-hydroxynaphthaldehyde
 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.*