Third Semester: Inorganic Chemistry

Subjects	Course Code	Credit Hours	Full Marks	Pass Marks
Inorganic Reaction Mechanism, Techniques and Inorganic Polymers	CHE-601	4	100	50
Selected Topics in Inorganic Chemistry	CHE-602	4	100	50
Inorganic Chemistry Practical	CHE-603a	5	125	62.5
Inorganic Chemistry Seminar	CHE-603b	1	25	12.5
Elective Papers	CHE-610 to 615	3	75	37.5

Third Semester: Physical Chemistry

Subjects	Course Code	Credit Hours	Full Marks	Pass Marks
Quantum Chemistry and Statistical Mechanics	CHE-604	4	100	50
Advanced Solid State Chemistry	CHE-605	4	100	50
Physical Chemistry Practical	CHE-606a	5	125	62.5
Physical Chemistry Seminar	CHE-606b	1	25	12.5
Elective Papers	CHE-610 to 615	3	75	37.5

Third Semester: Organic Chemistry

Subjects	Course Code	Credit Hours	Full Marks	Pass Marks
Organic Synthesis	CHE-607	4	100	50
Organic Reaction Mechanism	CHE-608	4	100	50
Organic Chemistry Practical	CHE-609a	5	125	62.5
Organic Chemistry Seminar	CHE-609b	1	25	12.5
Elective Papers	CHE-610 to 615	3	75	37.5

Elective Papers:

Subjects	Course Code	Credit Hours	Full Marks	Pass Marks
Food Chemistry	CHE-610	3	75	37.5
Natural Product Chemistry	CHE-611	3	75	37.5
Nuclear Chemistry	CHE-612	3	75	37.5
Spectroscopy	CHE-613	3	75	37.5
Biochemistry	CHE-614	3	75	37.5
Analytical Chemistry	CHE-615	3	75	37.5

Elective courses to be offered based on the available man power in the department/campuses.

Students have to complete literature review and proposal defense of M. Sc. Dissertation in third semester under the assigned supervisor.

Inorganic Chemistry

Course Title: Inorganic Reaction Mechanism, Techniques and Inorganic Polymers (Theory)
Course No.: CHE-601
Semester: Third (3^{rd})

Credit: Four (4) hrs.
Full Marks: 100
Pass Marks: 50

Course Objectives:

- To acquaint the students with different types of inorganic reaction mechanisms.
- To provide the knowledge of stability constant and its application in inorganic chemistry.
- To provide an advanced knowledge of inorganic polymers.

Course Contents:

Group A

Inorganic Reaction Mechanism A: Introduction, kinetics and mechanism: review on transition state theory, reactants, products, activated complex, activation energy, intermediate species, endothermic and exothermic reaction, nucleophile, crystal field stabilization energy (CFSE).

Reaction mechanism of type dissociative reaction mechanism and associative reaction mechanism, five coordinate intermediate and seven coordinate intermediate, labile, inert, introduction to redox reaction and ligand substitution reaction in metal complexes.

Redox Reaction: Electron transfer reaction, atom transfer reaction**,** electron tunneling mechanism, experimental results, inner and outer sphere mechanism (evidence for electron transfer), effect of ions on the rate, complementary two equivalent exchange, electron transfer through extended bridge, crystal field effect, Frank Condon principle, Marcus theory, orbital symmetry in electron transfer, photochemical reactions.

Inorganic Photochemistry: Redox reactions of metal complexes in excited states. Excited state electron transfer example using $[Ru(bipy)_3]^{2+}$ and related complexes. Role of spin orbit coupling, lifetimes of excited states in these complexes.

Group B

Inorganic Reaction Mechanism B:

Ligand Substitution Reaction: Introduction, operational approach to classification of substitution mechanisms, stoichiometric mechanism, intimate mechanism.

Ligand Substitution Reaction in Octahedral Complexes: Nature of substitution reaction, theoretical approach of substitution mechanism: inorganic nucleophilicity scales, the effect of electronic structure of central atom; kinetic application of crystal field theory: mechanism of substitution reaction of complexes of Co(III): (a) acid hydrolysis, (b) π-bonding dissociation reaction of octahedral complexes (c) base hydrolysis of Co(III) complexes (d) substitution without breaking the metal ligand bond, racemization-reaction.

Ligand Substitution Reaction in Square Planar Complexes: Reactions of Pt(II) complexes: the trans effect, trans effect theories (polarization theory, π-bonding theory, molecular orbital theory for σ and π trans effect).

Mechanism of Substitution: Kinetics of substitution reactions of Pt(II) complexes: trans effect, cis effect, effect of leaving group, effect of charge, steric effect, solvent effect, effect of nucleophiles, effect of catalyst on substitution reaction by Pt (II) complexes.

Group C

Determination of Stability Constants: Introduction of thermodynamic stability constant or formation constant of metal complex, overall stability constant, stepwise stability constant, stoichiometric stability constants.

Basic Principle: Kinetic and equilibrium approach, determination of concentration variables (total concentration, free concentration, secondary concentration variables), determination of η, calculation of free ligand concentration "a", properties involving intensive factors.

Methods for the Determination of Stability Constant of Mononuclear Complex: Job's method of continuous variation for the determination of stability constant, Yoe Jone's molar ratio method for the determination of stability constant, Bent and French method for the determination of stability constant, determination of concentration variables using competitive reaction; BAH system adopted by J. Bjerrum, Calvin and Wilson.

Experimental Methods for the Determination of Stability Constant: Potentiometric method, paper chromatographic method.

Spectral Techniques in Inorganic Complexes: Mossbauer spectroscopy, nuclear magnetic resonance (NMR) spectroscopy, electronic spin resonance (ESR) spectroscopy, nuclear quadrupole resonance (NQR) spectroscopy.

Group D

Inorganic Polymers:

Introduction: Homopolymers, heteropolymers, elemento-organic polymers: homosubstituted, heterosubstituted and hybrid polymers, addition polymerization, condensation polymerization, coordination polymerization, organometallic polymers.

Silicon Polymers:

Silicones: Introduction, preparation, properties, a brief description of various types of silicones (silicone fluids, silicone rubber, silicone resins, higher polymer organosiloxanes etc.) and uses of silicones.

Polysilanes, silicon carbides.

Phosphorous Polymers: Condensed phosphates: metaphosphates, polyphosphates, long chain polyphosphate and cross linked phosphates, phosphorous nitrogen polymers (phosphonitrilic polymers).

Sulphur Polymers: Tetra sulphur tetra nitride, polythiazyls.

Applications of inorganic polymers

Reference Books for CHE-601:

1. F. Basolo and R. Pearson, *Mechanisms of Inorganic Reactions, A Study of Metal Complexes in Solution*, (2^{nd} Edition), Wiley Western Limited.
2. R.B. Jordan, *Reaction Mechanisms of Inorganic and Organo Metallic Systems*, (3^{rd} Edition) Oxford University Press New York, 1991
3. B. Douglas, D. McDaniel, J. Alexander, *Concepts and Models of Inorganic Chemistry*, John Wiley & Sons, Inc., 1994.
4. J.E. Huheey, Ellen A. Keiter and Richard L. Keiter, *Inorganic Chemistry*, (4^{th} Edition), Addition-Wishley Publishing Company, 1993.
5. W.U. Malik, Tuli G.D., and Madan R.D., *Selected Topics in Inorganic Chemistry, (*8^{th} Revised Edition), S. Chand and Company Pvt. Ltd., 2014.
6. Francis J.C. Rossotti and Hazel Rossotti, *Determination of Stability Constants*, McGRaw Hill.
7. Ebsworth F.A.O., *Structural Methods in Inorganic Chemistry*, Blackwell Scientific Publication, 1991.
8. R.G. Wilkins, *The Study of Kinetics and Mechanisms of Reactions of Transition Metal Complexes*, (2^{nd} Edition),V.C.H. Publishers, 1991.
9. H. Taube, *Electron Transfer Reactions of Complex Ion in Solution*, Academic Press, New York, 1970.

10. C.H. Langsford and H.B. Gray, *Ligand Substitution Processes*, Benjamin Commings, 1966.
11. J.O. Edward, *Inorganic Reaction Mechanisms*; Wiley-New York.
12. J. Lewis and R.G. Wilkins, *Modern Co-ordination Chemistry*, Interscience Publishers.
13. D. Katakis and G. Gordon, *Mechanism of Inorganic Reactions*, John Wiley and Sons, New York, 1987.
14. F.G.A. Stone and W.A.G. Graham, *Inorganic Polymers*, Academic Press, New York.
15. D.N. Hunter, *Inorganic Polymers*, Blackwell Scientific Publications, Oxoford.
16. H.J. Emeleus and A.G. Sharpe, *Modern Aspects of Inorganic Chemistry, (*4th Edition), Sixth Indian Reprint Universal Book Stall, New Delhi, 1992.
17. Eds M. Zelldin, K.J. Wynne and H.R. Allcock, ACS *Inorganic and Organometallic Polymers*, Symposium Series 360, American Chemical Society, Washington D.C., 1988.
18. J.E. Mark, H.R. Allcock and R. West, *Inorganic Polymers*, Prentice-Hall Englewood Clifts, NJ, 1992.
19. S. Pimplapure, A. Sahai, R. Jain, and U. Soni, *Inorganic Polymer Chemistry*, (1st Edition), Pragati Prakashan, 2012.

Inorganic Chemistry

Course Title: Selected Topics in Inorganic Chemistry (Theory) **Credit:** Four (4) hrs.
Course No.: CHE-602 **Full Marks:** 100
Semester: Third (3rd) **Pass Marks:** 50

Course Objectives:

- To acquaint the students with different types of inorganic reaction mechanisms.
- To provide knowledge of some specialized areas of inorganic chemistry and their applications.
- To give a comprehensive idea of the use of organometallic compounds.

Course Contents:

Group A

Inorganic Cage and Cluster and Compounds:

Cluster and Cage Compounds: Introduction, structure and bonding of boron hydrides, molecular orbital description of bonding in boron hydrides.

Heteroboranes: Carboranes, metalloboranes, metallocarboranes.

Chemistry of Boranes: Synthesis of boron hydrides.

Cluster Compounds: Clusters and catalysis, molecular structure of clusters, stereochemical non-rigidity in clusters, dynamic nuclear magnetic resonance spectroscopy, structures of clusters with π- acid ligands, metal carbonyl clusters, low-nuclearity (M_3 and M_4) clusters, isoelectronic and isolobal relationship, high nuclearity carbonyl clusters (HNCC), electron counting scheme for HNCC, HNCC'S of Fe, Ru and Os group, Co, Rh and Ir group and Ni, Pd and Pt group, Polyhedral Skeleton Electron Pair Theory (PSEPT) or Wade's Rule, the capping principle, structures not rationalized by the PSEPT model, halide clusters, synthesis of metal clusters, electron precise compounds and their relation to clusters, Polynuclear zintl anions and cations.

Group B

Solid State Material Chemistry: Synthesis of materials, defects and ion transport, solid electrolytes, solid oxide fuel cells, metal oxides, nitrides, fluorides, higher oxides and complex oxides, oxide glasses, chalcogenides, intercalation compounds and metal rich phases, chevrel phases and chalcogenide thermoelectrics. Framework structure, structure based on octahedral and tetrahedra. Hydrides and hydrogen storage materials, other inorganic hydrogen storage material. Inorganic pigments, Semiconductor chemistry,

Group 14 semiconductors, semiconductor system isoelectronic with silicon. Superconductors, molecular material and fullerides, molecular magnets, inorganic liquid crystals.

Group C

Organometallic Chemistry A:

Reviews on Organometallic Compounds: Introduction, classification based on the polarity of M-C bond, factors governing formation of C-H bonds, thermodynamic and kinetic stability of organometallic compounds, stability towards oxidation, stability towards hydrolysis.

Preparative routes for metal-carbon bond formation, miscellaneous methods of the preparation of the organometallic compounds.

Organometallic compounds of transition elements, σ-bonded organometallics, compounds with 1 electron ligand, compounds with 3 electron ligands, compounds with 5 electron ligands, π-bonded organometallics, compounds with 2 electron ligands, compounds with 4 electron ligand, compounds with 6 electron ligand, fluxinal organometallic compounds.

Group D

Organometallic Chemistry B:

Synthetic and catalytic aspects of organometallic chemistry, use of organo lithium, organo magnesium, organometallics of Zn, Cd, Hg in synthesis, use of organo copper, use of organo palladium compounds in synthesis. Homogenous and heterogenous catalysis involving organometallic compounds. Importance of transition metal in catalysis. Hydrogenation, hydroformylation ('oxo' process), Wacker process, use of Zeigler Natta catalyst, Fischer-Tropsch synthesis. Biological application and environmental aspects of organometallic chemistry.

Reference Books for CHE-602:

1. B. Douglas, D. McDaniel, J. Alexander, *Concepts and Models of Inorganic Chemistry*, John Wiley & Sons, Inc., 1994.
2. D.F. Shriver and P.W. Atkins, *Inorganic Chemistry*, (5th Edition) Oxford University Press.
3. F.A. Cotton, G. Wilkinson,C.A. Murillo and Manfred Bochmann *Advanced Inorganic Chemistry*, (6th Edition), John Wiley and Sons, 1999.
4. G.E. Coates M.L.H. Green, P. Powell and K. Wade, *Principles of Organometallic Chemistry*, Chapman and Hall, London, 1997.
5. I. Haiduc and J.J. Zuckermann, *Basic Organometallic Chemistry*, Walte de Gruyter, NY, 1985.
6. G. Wilkinson, F.G.A. Stone and E.W. Abel (Eds), *Comprehensive Organometallic* Chemistry, Pergamon Press, New York, 1982.
7. C. Masters, *Homogenous Transition Metal Catalysis*, Chapman and Hall, London, 1981.
8. J. P. Collman, L.S. Hegedus, J.R.; Norton and R.G. Finke, *Principles and Applications of Organotransition Metal Chemistry*, (2nd Edition), University Science Books, California, 2000.
9. R. C. Mehrotra and A. Singh, *Organometallic Chemistry (A Unified Approach)*, Wiley Estern Limited, 2000.
10. F. A. Cotton, G. Wilkinson and P. L. Gaus, *Basic Inorganic Chemistry*, (6th Edition), John Wiley and Sons, 1995.
11. J. E. Huheey, E.A. Keiter and R.L. Keiter, *Inorganic Chemistry*, (4th Edition). Harper-Collins,1993.
12. W.U. Malik, Tuli G.D., and Madan R.D., *Selected Topics in Inorganic Chemistry*, (8th Revised Edition), S. Chand and Company Pvt. Ltd., 2014.

Relevant articles from Progress in Inorganic Chemistry, Advances in Organometallic Chemistry will be used.

Inorganic Chemistry

Course Title: Inorganic Chemistry (Practical) **Credit:** Five (5) hrs.
Course No.: CHE-603a **Full Marks:** 125
Semester: Fourth (3^{rd}) **Pass Marks:** 62.5

Course Objectives:

- To acquaint the students with quantitative and qualitative analytical methods.
- To familiarize students with the techniques of preparation and with characterization of coordination compounds.

Course Contents:

Preparation:

1. Preparation of potassium trioxalato ferrate and estimation of percentage of oxalate and iron in the prepared complex. Compare the IR spectrum with potassium oxalate or oxalic acid.
2. Preparation and characterization of copper oxalate complex.
3. Preparation and characterization of cis and trans potassium dioxalato diaquo chromate (III).
4. Preparation and characterization of nitrito pentamine cobalt (III) nitrate.

Volumetric Analysis:

1. Determination of copper and cadmium in a mixture volumetrically and gravimetrically.
2. Determination of ferrous and ferric ion in a mixture by ceric salt.
3. Determination of amount of Manganese, Magnesium and Zinc in a mixture by using EDTA.
4. Analysis of low melting Bismuth-Lead-Cadmium-Tin alloy by using EDTA.

Salt Analysis:

1. Qualitative analysis of inorganic salt mixture involving 8 radicals by semimicro method (including interfering radical and rare earth).
2. Spot test analysis for inorganic cations and anions.

Instrumental Analysis:

3. Determination of composition of complex by Job's method.
4. Determination of stability constant.
5. Ion exchange chromatography.

Any other experiments to be introduced in class work during the semester.

Reference Books for CHE-603a:

1. I. Vogel, *A Text Book of Quantitative Inorganic Analysis, Including Elementary Instrumental Analysis*, ELBS & Longman, 1969, (Preferably available recent edition).
2. Angelici, *Synthesis and Technique in Inorganic Chemistry*; W.B. Sounders Co. (Sounders Golden Series), Philadelphia, 1991.
3. M.R. Pokhrel, P.N. Yadav and S. Shrestha, *Advanced Practical Inorganic Chemistry* for M.Sc., (2^{nd} Edition), Kshitiz Publication, 2017.
4. W.G. Palmer, *Experimental Inorganic Chemistry*, Cambridge University Press, UK (Preferably recent edition).
5. K. N. Ghimire, M. R. Pokhrel & K. P. Bohara, *University Experimental Inorganic Chemistry*, Quest Publication, Kirtipur, Kathmandu, 2008.

Inorganic Chemistry

Course Title: Inorganic Chemistry Seminar
Course No.: CHE-603b
Semester: Third (3^{rd})

Credit: One (1) hr.
Full Mark: 25
Pass Mark: 12.5

General instruction for the seminar: Students should collect at least five papers from peer reviewed journals published within last ten years. They will select one major peer reviewed paper of their choice to present in the seminar. Total time allocated for seminar must be 15 minutes including discussion.

Physical Chemistry

Course Title: Quantum Chemistry & Statistical Mechanics (Theory)
Course No.: CHE-604
Semester: Third (3^{rd})

Credit: Four (4) hrs.
Full Mark: 100
Pass Mark: 50

Course Objectives

- To learn the rules of quantum chemistry, do calculations and discuss the concepts.
- To provide the basic knowledge of statistical mechanics.

Course Contents:

Group A

Basics of Quantum Mechanics: Review of postulates of quantum mechanics; time dependent Schrödinger wave equation; poisson bracket and commutator bracket; orthonormal basis; closure relation; linear independence; linear operators; vector interpretation of wave function; linear vector space; theorems of vector spaces; matrices and quantum mechanics; transmission coefficient of a particle from a potential barrier; quantum mechanical tunneling and its applications; quantum mechanical virial theorem and its applications; Heisenberg's uncertainty principle; Heisenberg equation of motion.

Group B

Harmonic Oscillator: Harmonic oscillator (eigen value, wave function; selection rule and calculation); significant of zero point energy; recursion relation; Hermite polynomials.

Quantum Theory of Angular Momentum and Rigid Rotator: Review of classical angular momentum; commutation properties of the angular momentum operators; angular momentum in spherical polar coordinates; ladder operators; eigenvalues of $\hat{L}_z$ and $\hat{L}^2$; rigid rotator (eigen value, wavefunction, selection rule and calculations).

Group C

Approximate Solutions to Schrödinger Equation: Variation method (Rayleigh-Ritz method) and its applications (particle in a box, hydrogen and helium atom); mass polarization effect; secular determinant; perturbation theory for nondegenerate ((Rayleigh-Schrödinger and variational methods) and degenerate states; time-dependent perturbation theory and its application in time-domain spectroscopy; application of perturbation theory (He and Stark effect).

Hartree and Hartree-Fock Self-Consistent Field Method: Hartree and Hartree-Fock self-consistent field methods; density matrix analysis of the Hartree-Fock approximation; matrix solution representation of the Hartree-Fock equations (Roothaan's equations).

Introduction to molecular Structure: Born-Oppenheimer approximation, molecular Hartree-Fock calculations.

Group D

Statistical Mechanics: Review lecture of phase space and ensemble; Liouville's theorem, statistical equilibrium; postulates of equal probability; principle of equipartition of energy.

Quantum statistics: Introduction; Bose-Einstein statistics; statistics and condensation; thermodynamic properties of ideal Bose-Einstein gas; Fermi-Dirac statistics; degenerate Fermi gas; comparison of Bose-Einstein; Fermi-Dirac and Maxwell-Boltzmann statistics; application of quantum statistics.

Partition function: Translational; rotational; vibrational and electronic partition functions; Gibbs paradox; Sackur-Tetrode equation; applications of partition functions to specific heat of ideal gas; solid and chemical equilibrium.

Reference Books for CHE-604:

1. F. L. Pilar, *Elementary Quantum Chemistry*, (2nd Edition), Dover Publications, New York, USA, 1990.
2. P. Atkins and R. Friedman, *Molecular Quantum Mechanics*, (8th Edition), Oxford University Press, New York, USA, 2009.
3. I. N. Levine, *Quantum Chemistry*, (6th Edition), PHI Learning Pvt. Ltd., New Delhi, 2012.
4. J. M. Andersen, *Introduction to Quantum Chemistry*, Benjamin, New York, 1969.
5. H. Eyring, J. Walter and G. E. Kimball, *Quantum Chemistry*, John Wiley & Sons, Inc., London, 1960.
6. J. P. Lowe, *Quantum Chemistry*, (2nd Edition), Academic Press California, 1993.
7. V. K. Jha, *Introductory Quantum Mechanics*, Kathmandu, Nepal, 2012.
8. A. K. Chandra, *Introductory Quantum Chemistry*, (4th Edition), Tata McGraw-Hill, New Delhi, India, 1994.
9. Y. R. Waghmare, *Introductory Quantum Mechanics*, Eurasia Publishing House, New Delhi, India, 1989.
10. B. S. Rajput, *Advanced Quantum Mechanics*, (9th Edition), Pragati Prakashan, Meerut, India, 2009.
11. R. K. Prasad, *Quantum Chemistry*, (2nd Edition), New Age International Publication, New Delhi, India, 2000.
12. S. Glasstone, *Theoretical Chemistry*, (1st Edition), D. Van Nostrand Company, Inc., New York, 1944.
13. S. L. Gupta, V. Kumar, *Elementary Statistical Mechanics*, (23rd Edition), Pragati Prakashan, India (2009).
14. B. K. Agrawal, M. Eisner, *Statistical Mechanics*, John Wiley and sons (1988).

Physical Chemistry

Course Title: Advanced Solid State Chemistry (Theory) **Credit:** Four (4) hrs.
Course No.: CHE-605 **Full Mark:** 100
Semester: Third (3rd) **Pass Mark:** 50

Course Objective:

- To provide the advance knowledge of solid state and advanced materials chemistry.

Course Contents:

Group A

Imperfections in Solids: Defects in solids; point defects: vacancy in elemental solids; Schottky defects in ionic crystals; self-interstitial in elemental solids; Frenkel defects in ionic solids; interstitial impurity in

metals, vacancy through alliovalent impurity in ionic solids; charge compensation in ionic solids; color centers; diffusion in solids: mechanism, steady and non steady state diffusions, affecting factors for diffusion; ionic conductivity and super ionic conductivity.

Group B

Electrons in Solids: Quantum mechanical free electron theory; Fermi energy and Fermi distribution function; density of states; band theory; the hole concept; semiconductors; extrinsic semiconductivity and temperature variation of electrical conductivity.

Solid State Reactions: Wagner's theory; oxidation of metals; kinetics of oxide film growth and photographic process.

Group C

Super Conductivity: Occurrence of superconductivity; Meissner effect; BCS-theory of superconductivity; high temperature superconductivity; critical field and critical currents; organic superconductors and fullerenes, new superconductors, applications of superconductors.

Preparation of Materials: Crystal growth: general consideration; growth from vapor; growth from melt; growth from solid-state reaction; crystallization from solution; materials purification: zone refining.

Group D

Advanced Materials Chemistry: Introduction; classification of materials; *Composition and microstructure of iron-carbon alloys:* formation of ferrite; austenite and cementite phases in iron with iron-iron carbide phase diagram; microstructure development in iron-carbon alloys; *phase transformations*: basic concepts; kinetics of phase transformations; micro-structural and property change in iron-carbon alloys with isothermal and continuous cooling transformation diagrams; mechanical behavior of iron-carbon alloys.

Some solid materials of importance: semiconductor devices: p-n rectifying junction; transistor; microelectronic circuitry; integrated circuit of aluminum; capacitors; magnetic storage devices; shape-memory alloys; carbon nano-tubes; light-emitting diodes; optical fibers in communications.

Reference Books for CHE-605:

1. S. O. Pillai, *Solid State Physics*, Wiley Eastern Ltd., New Delhi, 1994.
2. H. V. Keer, *Principles of the Solid State*, New Age Inlt. Ltd., New Delhi, 2002.
3. C. Kittel, *Introduction to Solid State Physics*, (8^{th} Edition), John Wiley & Sons Inc., NJ, 2004.
4. N. B. Hannay, *Solid State Chemistry*, Prentice-Hall of India, New Delhi, 1976.
5. D. K. Chakrabarty, *Solid State Chemistry*, New Age Int. Ltd., New Delhi, 1996.
6. P. Atkins and J. de Paula, *Atkins' Physical Chemistry*, (10^{th} Edition), Indian edition, Oxford University Press, 2014.
7. W. D. Callister Jr. and D. G. Rethwisch (adopted by R. Balasubramaniam), *Callister's Materials Science and Engineering*, Wiley India Pvt. Ltd., New Delhi, 2010.
8. C. R. Barrett, W. D. Nix and A. S. Tetelmann, *The Principles of Engineering Materials*, (1^{st} Edition), Prentice-Hall Inc, New Jersey, 1973.
9. W. F. Smith and J. Hashemi, *Foundation of Materials Science and Engineering*, (4^{th} Edition), McGraw-Hill, 2006.
10. V. Raghavan, *Materials Science and Engineering: a First Course*, (5^{th} Edition), PHI Learning Pvt. Ltd., New Delhi, 2011.

Physical Chemistry

Course Title: Physical Chemistry Practical
Course No.: CHE-606a
Semester: Third (3^{rd})

Credit: Five (5) hrs.
Full Mark: 125
Pass Mark: 62.5

Course Objective:

- To acquaint the student with advanced experimental techniques on physical chemistry.

Course Contents:

Electrochemistry

1. Estimation of mineral acid impurity in a commercial sample of vinegar by conductance measurement.
2. Determination of the composition of zinc ferrocyanide precipitates on addition of zinc sulphate to acidified potassium ferrocyanide solution potentiometrically.
3. Construction of silver/silver chloride reference electrode and determination of its electrode potential.
4. Determine two pKa values of glycine by titration method.

Chemical Kinetics

5. Hydrolysis of an ester catalyzed by enzyme α-chymotrypsin.
6. Determination of activation energy for the reaction between potassium persulphate and iodine with and without catalyst.
7. Kinetic study of the reaction between acetone and iodine in presence of mineral acid as catalyst and find out order with respect to (a) iodine and (b) acetone and (c) acid.

Colorimetry/Spectrophotometry

8. Kinetics of iodination of acetone by colorimetric method.
9. Determination of dissociation constant of indicator by spectrophotometric method.
10. Kinetic study for iodination of cyclohexanone in acidic medium by colorimetric method.

Miscellaneous

11. Determination of coordination number of copper in copper-ammonia complex by distribution method.
12. Experiments on gas chromatography.
13. Determination of micelle concentration (CMC) of a common detergent and study the effect of salt on the CMC by conductometrically.
14. A particle in a box laboratory experiment using everyday compounds.

Any other experiments to be introduced in class work during the semester.

Reference Books for CHE-606a:

1. J. N. Gurtu and A. Gurtu, *Advanced Physical Chemistry Experiments*, (6^{th} Edition), Pragati Prakashan, Meerut, India, 2014.
2. *Findlay's Practical Physical Chemistry*: (9^{th} Edition), revised by B. P. Levitt, Longman Group Ltd., London, 1973.
3. H. A. Neidig, W. J. Straton (Compiled), *Modern Experiments for Introductory Chemistry* [Reprint from Journal of Chemical Education, Wiley Eastern Ltd., New Delhi, 1994.
4. Advanced Physical Chemistry Laboratory Manual, P. S. Phillips, 2010.
5. T. Wimpfheimer, A particle in a box laboratory experiment using everyday compounds, *Journal of Laboratory Chemical Education*, 3(2), 19-21, 2015.

Physical Chemistry

Course Title: Physical Chemistry Seminar
Course No.: CHE-606b
Semester: Third (3^{rd})

Credit: One (1) hr.
Full Mark: 25
Pass Mark: 12.5

General instruction for the seminar: Students should collect at least five papers from peer reviewed journals published within last ten years. They will select one major peer reviewed paper of their choice to present in the seminar. Total time allocated for seminar must be 15 minutes including discussion.

Organic Chemistry

Course Title: Organic Synthesis (Theory)
Course No.: CHE-607
Semester: Third (3^{rd})

Credit: Four (4) hrs.
Full Marks: 100
Pass Marks: 50

Course Objective:

- To enable the students to obtain advanced knowledge in methods, design, logic and analysis in synthetic organic chemistry

Course Contents:

Group A

Extensive Study and Applications Modern Synthetic Reactions:

a. Reduction
b. Oxidation
c. Halogenation and alkylation
d. Acylation, aldol condensation and related reactions

Group B

Organic Synthesis: Types of synthesis (classical, rational, partial, total, commercial); nature of synthesis (laboratory, asymmetric, stereoselective, chemo and regio-selective, chiral, biomimetic, symmetry based synthesis, biosynthesis and biogenesis, ideal or perfect synthesis).

Synthetic Tools and Reagents: synthetic planning and synthetic design; the principles of synthesis, synthetic process & steps in synthesis; carbon framework construction and functional group modification; key intermediates; starting materials; linear & convergent approach; relay approach, blocking groups, protecting groups, masking groups.

Group C

Modern Synthetic Concepts: Retrosynthetic analysis and disconnection approach, basic principles,one group disconnection and two group disconnection, synthon and synthetic equivalent, retron and transforms, reversal of polarity, functional group interconversion, order of events in organic synthesis, amine synthesis, and control in carbonyl condensation.

Total Synthesis of Compounds: Tropenone, Cholesterol, Longifolene, Penicillin, Prostaglandin E_2 and Taxol

Group D

Organometallics in Organic Synthesis: Synthetic uses of organometallic compounds obtained from boron, silicon, selenium, copper and transition metals.

Metathesis Reactions: Introduction to metathesis, type of metathesis reaction, Schrock's and Grubb's catalysts, catalytic cyclic mechanism, reaction scope and condition, synthetic applications.

Pd-Catalyzed Cross Coupling Reaction: Cross-coupling reactions, Pd-catalyzed cross-coupling reactions, mechanism, Heck, Negishi and Suzuki Pd-catalyzed cross-coupling reactions and their mechanism, synthetic applications.

Reference Books for CHE-607:

1. R. E. Ireland, *Organic Synthesis*, Prentice Hall, 1969.
2. E. J. Corey: *The Logic of Chemical Synthesis*, John Wiley and Sons NK, 1989.
3. S. Hamessian, *Total Synthesis of Natural Products, Chiron Approach*, Pregmon Press, Oxford 1983.
4. H. O. House, *Modern Synthetic Reactions*; W.A. Bezamin, New York, 1972.
5. I. Fleming, *Selected Organic Synthesis*, John Wiley and Sons, 1973.
6. K. C. Nicolaou and E.J. Sorensen, *Classics in Total Synthesis*, VCH Germany, 1996.
7. A. J. Chichester, *Organometallic Compounds*, John Wiley, 1985.
8. J. H. Swan and D. St. C. Black, *Organometallics in Organic Synthesis,* London, Chapman and Hall, 1985.
9. R. Norman and J. M. Coxon, *Principles of Organic Synthesis*, CRC/CBS Publishers & Distributors, 1993.
10. H. Waldmann, *Organic Synthesis Highlights,* VCH, Germany, 1995.
11. S. Warren, *Organic Synthesis, The Disconnection Approach*, Wiley, New York, 1982.
12. M. B. Smith, Organic Synthesis, (3rd Edition), McGraw-Hill Companies, 1994.
13. I. Kumar, Organometallic Compounds, Pragati Prakashan, Meerut, India, (5th Edition), 2015.

Organic Chemistry

Course Title: Organic Reaction Mechanism (Theory) **Credit:** Four (4) hrs.
Course No.: CHE-608 **Full Marks**: 100
Semester: Third (3rd) **Pass Marks**: 50

Course Objective:

- To acquaint the students with major types of reaction mechanisms encountered in organic chemistry.

Course Contents:

Group A

Aliphatic Nucleophilic Substitution: Introduction and review,reactivity, the effect of substrate structure, the effect of attacking nucleophile, the effect of the leaving group, the effect of reaction medium phase transfer catalysis and ultra sound, ambident nucleophiles, regioselectivity, eight mechanisms of ester hydrolysis, typical reactions with mechanisms.

Aromatic Nucleophilic Substitution: Review, reactivity, the effect of substrate structure, the effect of the leaving group, the effect of the attacking nucleophile, typical reactions with mechanisms.

Aromatic Electrophilic Substitution: Review, orientation in benzene rings with more than one substituent, orientation in other ring systems, quantitative treatments of reactivity in the substrate, the selectivity relationship, the effect of the leaving group, typical reactions with mechanisms.

Aliphatic Electrophilic Substitution: Review, electrophilic substitution accompanied by double bond shifts, reactivity effect of substrate, effect of leaving group, effect of solvent, typical reactions with mechanisms.

Group B

Free Radical Substitution: Review, mechanisms at an aromatic substrate, reactivity for aliphatic substrate, reactivity in aromatic substrate, reactivity in the attacking radical, the effect of solvent on reactivity, typical reactions with mechanisms.

Addition to Carbon–Carbon Multiple Bonds: Review, orientation and reactivity – reactivity, orientation, stereochemical orientation, typical reactions with mechanisms.

Addition to Carbon–Hetero Multiple Bonds: Review, mechanism and reactivity, typical reactions with mechanisms.

Rearrangements: Review, nucleophilic rearrangements, the actual nature of the migration, migratory aptitudes, memory effects, longer nucleophilic rearrangements, free radical rearrangements electrophilic rearrangements and reactions involving carbon to oxygen migrations, typical reactions with mechanisms.

Group C

Reactive Intermediates: Carbenes, structure and generation, Bamford-Stevens reaction, Seyferth and coworker's method, trihalocarbonyl reaction, proplysis of the salts of trihaloacetic acid, reaction of RLi with alkyl halide, Simmons Smith reaction structure, conversion of singlet to triplet state, stererospecific and nonsterospecific reactions of triplets, insertion reactions, halomethylation, problems.

Nirenes: Generation- Rearrangement, migration to carbon, migration to nitrogen, stereospecific and nonstereospecific reactions, insertion reaction, fragmentation reactions, problems.

Ylids and Related Chemistry: Generation of phosphoniummethylides, phosphonatecarbanion and their reactions, generation of sulfonium and sulfoxoniummethylide and their reactions,sulphur- ylide.

Group D

Conservation of Orbital Symmetry: Pericyclic reaction, conservation of electrocyclic reactions, stereochemistry molecular orbital symmetry, symmetry control of electrocyclic reactions, sigmatropic reactions, examples of the stereochemistry of sigmatropic reactions, and alternate qualitative molecular orbital approach (Frontier molecular orbital method).

Classification of cycloaddition process, orbital symmetry and cycloaddition, concerted vs.nonconcertedcycloaddition, $\pi 2 + \pi 2$ cyloaddition, $\pi 2 + \pi 4$ cyloaddition, diene component of the Diels-Alder reaction, dienophile-reactivity, stereochemistry of the Diels–Alder reaction.

References Books for CHE-608:

1. J. March, *Advanced Organic Chemistry,* (4^{th} Edition), John Wiley and Sons, 1992.
2. C. H. DePuy and Orville L. Chapman, *Molecular Reactions and Photochemistry,* Prentice-Hall of India Pvt. Ltd., 1975.
3. E. S. Gould, *Mechanism and Structure in Organic Chemistry*, Holt, Reinhart and Winstron, 1963.
4. Von R. Breslow, *Organic Reactions Mechanism,* W.A. Benjam Inc., NY, 1965.
5. M. Jones and R.A. Moss and M. S. Platz (editors), *Reactive Intermediates Chemistry*, John Wiley and Sons, Inc., 2003.
6. R. B. Woodward and R. Hoffmann, *Conservation of Orbital symmetry*, Verlag Chemie GmbH, Academic Press, 1971.
7. P. Skyes, *A Guide Book to Mechanism in Organic Chemistry,* Orient Longman, 1986.
8. W. J. Le Noble, *Highlights of Organic Chemistry,* Marcel Dekker, Inc. 1974.
9. C. K. Ingold, *Strucuture and Mechanism in Organic Chemistry*, Cornell University Press 1957.
10. L. F. Fieser and M. Fieser, *Organic Chemistry*, Reinhold Publishing Corporation, 1960.

Organic Chemistry

Course Title: Organic Chemistry Practical
Course No.: CHE-609a
Semester: Third (3rd)

Credit: Five (5) hrs.
Full Marks: 125
Pass Marks: 62.5

Course Objective:

- To equip the students with the techniques of separation, identification, isolation and estimation of organic compounds as well as with the techniques of handling various types of equipment's.

Course Contents:

1. Separation of organic mixtures based on solubility. Separation of the following organic mixtures (solid-solid, solid-liquid and liquid-liquid) based on solubility involving the following reagents (10% aqueous solution of $NaHCO_3$, NaOH and HCl) as well as with water or ether or saturated solution of $NaHSO_3$. Purification of separated compound is essential and is to be checked by TLC and melting point determination.
2. An experiment on chemical kinetics (titrimetric method)
3. Determination of specific rotation to study the inversion of cane sugar.
4. An experiment using flame photometer.
5. An experiment based on the chemical kinetics by spectrophotometric method.
6. An experiment on molecular weight determination (Rast method) and volumetric method.

Any other experiments to be introduced in class work during the semester.

Reference Books for CHE-609a:

1. N. K. Vishnoi, *Advanced Practical Organic Chemistry*, (2nd Revised Edition), Vikas Publishing Pvt. Ltd, 1996.
2. A. I. Vogel, *A Text Book of Practical Organic Chemistry*, (5th Edition), Longman, 1989.
3. R. L. Shriner, R. C. Fuson and D. Y. Curtin and T. C. Morrill, *The Systematic Identification of Organic Compounds*, (6th Edition), John Wiley & Sons, 1980.

Organic Chemistry

Course Title: Organic Chemistry Seminar
Course No.: CHE-609b
Semester: Third (3rd)

Credit: One (1) hr.
Full Mark: 25
Pass Mark: 12.5

General instruction for the seminar: Students should collect at least five papers from peer reviewed journals published within last ten years. They will select one major peer reviewed paper of their choice to present in the seminar. Total time allocated for seminar must be 15 minutes including discussion.

Elective Paper

Course Title: Food Chemistry (Theory) **Credit:** Three (3) hrs.
Course No.: CHE-610 **Full Marks:** 75
Semester: Third (3rd) **Pass Mark:** 37.5

Course Objective:

- To provide the students the basic knowledge on the composition, structure and properties of food and the chemistry of changes occurring during process and utilization.

Course Contents:

Group A

Recent development in food chemistry and its scope in food technology, chemical composition of food and classification, food as source of nutrients, moisture in food, Physical properties of water and ice, sorption phenomena, types of water free and bound water, water activity and its significant, solution and the colloidal state in food.

Carbohydrates: glycosides, action with alkali upon sugar, reducing action of sugar in alkaline solution, colour reaction of carbohydrate, sugar derivatives of biological importance.

Disaccharides: Properties and uses of maltose and lactose. Polysaccharides: homopolysaccharides: structure and properties of cellulose and starch, refining process of starch from dent corn, gelatinization, retrogradation of starch, modified starch and their application, manufacture of glucose syrup (corn syrup), structure, general properties and industrial applications of glycogen, dextrin and insulin.

Heteropolysaccharides: constituents and differences between cellulose and hemicellulose, partial structure of wheat flour hemicellulose, gums and mucilages, classification of gums, some important gums and their chemistry (gum arabic, guar gum), seaweed polysaccharides (agar, alginates, carageenan), chemical modification (cross–linking, substitution with stabilizing functional group and cleavage)

Vitamins: Introduction, water soluble vitamins: thiamin (vitamin B1), riboflavin (vitamin B2), ascorbic acid (vitamin C): Physiological role in human body, deficiency, diseases, functions, recommended dietary allowances (RDA) and loss in food processing, fat soluble vitamins: vitamin A (retinol), vitamin D (calciferol): Physiological role in human body, deficiency, diseases, functions, recommended dietary allowances (RDA) and loss in food processing.

Minerals: occurrence, minerals in plant products, minerals in meat, metal up taken in canned foods, biochemical functions and nutritional aspect of the major salt components in terms of functions, deficiency problems and excess amount: sodium (Na) and nickel (Ni).

Group B

Pectin: occurrence, chemical structure, classification, role of pectolytic enzymes, theories of gel formation and uses of pectin (e.g. Jam, Jelly and marmalades), Jelly grade, setting time.

Proteins: essential amino acids, chemical properties, peptide bond (geometry), zwitter ion, isoelectric point, colour reaction (ninhydrin reaction, biuret test, xanthoproteic reaction, Maillon reaction), synthesis of simple peptide (general chemical method), denaturation, estimation of protein by Kjeldahl method and formal titration (Sorensen method), meat proteins constituents, ageing of meat (rigor mortis), tenderization of meat (proteases), milk protein composition, wheat protein composition and leavening character.

Pigments and Color: natural pigments, occurrence and chemistry of chlorophyll, carotenoid, flavonoids and anthocyanin, effect of processing or during cooking of these pigments.

Synthetic Color: coal tar dye, safety and regulation, permitted food color, food drugs and cosmetic act (FDC).

Adulteration of Food: adulteration of food with suitable common examples such as oil, sugar, honey and milk, some examples of analytical methods of detection, basic principle of food preservation: traditional and synthetic food preservatives.

Group C

Enzymes: modern concept of mechanism of enzyme reaction, activity of food enzymes in different foods, blanching, application of enzymes in the food industries (amylase, proteases, lipase, glucose-oxidases), inhibition: competitive and non-competitive inhibition, Immobilized enzymes.

Lipids: introduction, identification of natural fats and oils, Phospholipids, role of phospholipids in biological system, photooxidation of lipids, flavor reversion, structure, properties and uses of lecithin, refining of vegetable oil, hydrogenation of vegetable ghee and margarine, rancidity types (oxidative rancidity and hydrolytic rancidity), mechanism and preventive measure of rancidity (using synthetic and natural antioxidants).

Browning in Foods: browning reaction, enzymatic browning, prevention of enzymatic browning, non-enzymatic browning types (maillard browning, caramelization and ascorbic acid browning), mechanism and method of prevention, food additives: introduction, a) non-nutritive sweetener (aspartame, saccharin, cyclamate, dihydrochalcon. b) emulsifier-principle giving with suitable examples c) stabilizer and thickening agent-their function with suitable examples d) antioxidants-natural and synthetic antioxidants with their mechanism of prevention e) natural colorants-caramel, lycopene, curcumin, crocin (saffron).

Flavour and Texture: sensation of taste and odour, substances with taste, flavour compounds (terpenoids, flavonoids, sulphur compounds, flavor inhancer (monosodium glutamate MSG), synthetic flavoring substances, texture improving additives, applications to food particularly with reference to fruits.

Reference Books for CHE-610:

1. L. H. Meyer, *Food Chemistry,* (1st Indian Edition), CBS Publisher and Distributors, 1987.
2. J. B. S. Braverman, *Introduction to the Biochemistry of Foods*, Elsevier Science Ltd. 1976.
3. Frank A. Lee, *Basic Food Chemistry*, Avi Publishing Company, 1983.
4. J. L. Jain, *Fundamentals of Biochemistry*, (6th Edition), S. Chand and Company Ltd. 2005.
5. G. G. Birch, L. F. Green and C. B. Coulson (eds.), *Sweetness and Sweeteners*, Applied Science, 1971.
6. O. R. Fennema, *Food Science part 1*, Food Chemistry, 1996.
7. N. S. Manay and M. Shadaksharaswamy, *Foods Facts and Principles,* New Age International Publishers, 2013.
8. N. Pennington and C. W. Baker, *Sugar Users Guide to Sucrose*, Chapmann and Hall, London. New York, 1990.
9. L. W. Aurand and A. E. Woods, *Food Chemistry*, The AVI publishing Co., Connectint, 1973.
10. E. A. Davidson, *Carbohydrate Chemistry*, Holt, New York, 1967.
11. N. N. Potter and J. H. Hotchkiss, *Food Science*, CBS Publisher and Distributors, 1996.
12. J. M. de Man, *Principles of Food Chemistry,* (3rd Edition), A Chapman and Hall Food Science Book, Aspen Publisher, 1999.

Elective Papers

Course Title: Natural Products Chemistry (Theory) **Credit:** Three (3) hrs.
Course No.: CHE-611 **Full Marks:** 75
Semester: Third (3^{rd}) **Pass Marks:** 37.5

Course Objective:

- To provide broad knowledge on synthesis, biosynthesis of molecules of nature and the techniques for their structure elucidation.

Course Contents:

Group A

Background and character of natural product chemistry, history and reference of natural products chemistry, definition and classification of natural products based on chemical, physiological activity and taxonomy, phytochemical techniques, extraction, isolation, purification and characterization of natural products.

Primary and secondary metabolism: Introduction, biogenesis of natural products, fatty acid biosynthesis, biosynthesis of polyacetylenes.

Biosynthetic Techniques: Introduction, isotopic labeling by radioactive isotopes and stable isotopes, enzyme and mutant.

Biosynthesis of the following:

Polyketides: Introduction, formation of poly β-keto acyl CoA's.

Terpenes and steroids: Introduction, steroids, pentacyclictriterpenes, squalenes, carotenoids, VitA.

The shikimic acid pathway: Introduction, quinines, coumarins and flavonoids.

Alkaloids: Introduction, morphine and related alkaloids.

Group B

Bio-assay techniques to screen the natural products, structure-activity relationship.

Medicinal Chemistry: Drug discovery, development and design.

Discovery, research and development of Taxol.

Discovery, development and structure of Quinghaosu.

General classification, extraction, isolation, purification of natural products and structure elucidation by chemical and spectroscopic methods and synthesis of the following:

Alkaloids: morphine, colchicines.

Terpenes and Steroids: Camphor, abietic acid, use of steroidal hormones and contraceptives (progestogen, ostrogen and their derivatives).

Anthocynins: Calistephin chloride.quercetin

Carbohydrates and Glycosides: Preparation of glycoside, chemical properties of glycosides, isolation, degradation, structure and application of heparin.

Group C

Isolation, structure elucidation and synthesis of the following:

Antibiotics: Cephalosporin C, chloromycetin, streptomycine.

Vitamin: Vitamin A, Vitamin B_1, B_{12}, Vitamin C.

Macromolecules: Natural rubber, resins, natural macrolides, fatty acids.

Naturally Occurring Organometallic Compounds: Chlorophyll and haemin.

Insecticides and related natural products: Classification, synthesis and uses of natural organic insecticides, (pyrethrines, rotenone), synthesis and uses of organic pesticides (organochlorine insecticide, organic fungicide, weedicides, pheromones, plant hormones, gibberellins, phytoalexins).

Reference Books for CHE-611:

1. N. R. Fransworth and A. S. Bingel, [H. Wagner and P. Walff (Eds)], *New Natural Products and Plant Drugs with Pharmacological, Biological or Therapeutical Activity*, springer, New York, 1976.
2. *Matthias Hamburger, Kurt Hostettmann Bioactivity in Plants: the link between phytochemistry and medicine*, Phytochemistry, Vol. 30, No 12, pp 3864 -74, 1991.
3. I. L. Finar, *Organic Chemistry;* Vols. I and II, ELBS Publication, 1975.
4. W. Herz Ed. *DGI Kingston's Progress in Chemistry of Natural Products,* Vol. 61, (G.W. Kirby, R. E. Moore *et al*.) Springer Verlag, 1993.
5. Kingston, D. G. I.; Magri, N. F.; Jitrangsri, C., Synthesis and Structure-Activity Relationships of Taxol Derivatives As Anticancer Agents, in *New Trends in Natural Products Chemistry*, Atta-ur-Rahman and LeQuesne, P.W., Ed.: Elsevier, Amsterdam, 1986.
6. N. Bodar, *Novel Approaches to Design Safer Drugs*, Academic Press, pp. 256-331 1984.
7. Nakanishi, *Natural Product Chemistry; Vols I, II and III,* Academi Press, 1975.
8. T. A. Geissman, DHG Crout, Freeman, *Organic Chemistry of Secondary Metabolism*, Freeman Cooper and Company, California, 1969.
9. R. B. Herbert, *Biosynthesis of Secondary Metabolism*, Chapman and Hill Ltd, 1981.
10. L. Dahal, *A Study on Pesticide Pollution in Nepal*, IUCN, NCS implementation project, 1995.
11. J. B. Harbone and Helga Mabry Ed, *The Flavonoids: Part I and II*, Chapmann and Hall 1980.
12. H. Schmutterer, K. R. S. Ascher Ed, *Natural Pesticides from The Neem Tree*, Proceedings of the First, Second and Third International Neem Conferences, Schriftenreihe der GTZ No.266, Eschborn,1987.
13. Human Medicinal Agents from Plants; American Chemical Society, Symposium Series 534, Washington DC, USA, 1993.
14. *Medicinal Plants in Nepal*, RDRL, Publication, HMG Nepal.
15. J. Singh, S. M. Ali, J. Singh, *Natural Products Chemistry*, (6^{th} Edition), Pragati Prakashan, Meerut, India, 2015.

Elective Paper

Course Title: Nuclear Chemistry (Theory)
Course No.: CHE-612
Semester: Third (3^{rd})

Credit: Three (3) hrs
Full Marks: 75
Pass Marks: 37.5

Course Objective:

- To Provide advanced knowledge on structure and composition of nuclei, radiochemistry, radiation chemistry, important nuclear reactions, radio-toxicity, and radiation biology.

Course Contents:

Group A

Nucleonics: Elementary particles and their classification, mass and charge of quarks, particles and anti-particles, quark-gluon interaction, properties of nuclei, size, shape and angular momentum of nucleus, principle and radial quantum numbers, nuclear parity and nuclear statistics, nuclear models- shell model, liquid-drop model and collective model.

Hot Atom Chemistry: Molecular disruption, Szilard-Chalmer's reaction, primary and secondary retention, different models for explaining recoil effects, thermal and gamma annealing.

Group B

Nuclear Reactions: Reaction cross-section, conservation in nuclear reactions, the compound nucleus theory, specific nuclear reactions due to neutrons, protons, deuterons, tritons, alphas and heavy ions, photonuclear reactions and transuraniens, symmetric and asymmetric fission and fission products, thermonuclear reactions, fission reactors, steller energy and cold fusion.

Radiation Biology: Biological effects of radiation, genetic effects of radiation, maximum permissible dose, effects of radiation in DNA and its constituents, nuclear magnetic resonance imaging (MRI) in medical diagnosis.

Group C

General Radiochemistry: Isotope exchange reactions, coprecipitation, colloids and adsorption of radioisotope, isotope dilution analysis, physical and chemical isotope effects.

Radiation Chemistry: Interaction of radiation with matter, dosimetry, radiolysis of water, radiolysis of benzene, autoradiolysis, time scale of radiolytic events, radiation hazards, classification of radiotoxicity, safety standards, radioactive waste disposal, environmental radioactivity.

Reference Books for CHE-612:

1. H. J. Arnikar, *Essentials of Nuclear Chemistry*, (4^{th} Edition), Wiley-Eastern Limited, 1995
2. C. Keller, *Radiochemistry*, Ellis Norwood Limited, 1988.
3. C. R. Choppin and J. Rydberg, *Nuclear chemistry: Theory and Applications*, Pergamon Press, 1980.
4. An. N. Nesmeyanov, *Radiochemistry*, Mir Publications, 1974.
5. A. K. Srivastava and P.C. Jain, *Elements of Nuclear Chemistry*, S. Chand and Company Ltd., 1983.
6. M. Haissainsky, *Nuclear Chemistry and its Applications*, Addison-Wesley Publishing Company, Inc., 1964.
7. G. Friedlander, J.W. Kennedy, E. S. Mahap and J.M. Miller, *Nuclear and Radiochemistry*, John-Wiley and sons, 1973.
8. E. J. Hall, *Radiation and Life*, Pergamon, 1984.
9. B. G. Harvey, *Nuclear Chemistry*, Prentice Hall, 1965.
10. H. A. C. McKey, *Principles in Radiochemistry*, Butterworths, 1971.
11. K. N. Rao and H. J. Arnikar, *Artificial Radioactivity*, Tata McGraw-Hill, 1986.
12. J. W. T. Spinks and R. J. Woods, *An Introduction to Radiation Chemistry*, John Wiley, 1976.
13. H. Kiefer and R. Maushart, *Radiation Protection Measurements*, Pergamon Press, 1972.
14. C. V. Sonntag Taylor and Francis, *The Chemical Basis of Radiation Biology*, 1987.

Elective Paper

Course Title: Spectroscopy (Theory)
Course No.: CHE-613
Semesters: Third (3^{rd})

Credit: Three (3) hrs.
Full Marks: 75
Pass Marks: 37.5

Course Objective:

- To provide advanced theoretical knowledge and information on the applications of different spectroscopic techniques.

Course Contents:

Group A

NMR Spectroscopy: *^{1}H-NMR*: The spinning nuclei, chemical shift and its measurement, factors affecting chemical shifts, anisotropic effect and shielding mechanism, interpretation of protons spin-spin coupling, coupling constant, simple, virtual and complex coupling, chemical and magnetic equivalence, first and non-first order spectra, analysis of AB, AMX and ABX systems, simplification of complex spectra and NOE deuterium exchange, hindered rotation and rate process, NMR studies of other nuclei e.g., ^{19}F, ^{31}P, ^{15}N and ^{11}B. Application in structural determination of simple organic and inorganic molecules; *^{13}C-NMR*: General introduction, peak assignments, chemical shift, ^{13}C-^{1}H coupling, off-resonance decoupling, deuterium, fluorine and phosphorus coupling, NOE and DEPT, 2D NMR, application to simple organic and inorganic molecules.

Electron and X-ray Spectroscopy: *Electron spectroscopy*- principle and applications of electron energy loss spectroscopy (EELS) and auger electron spectroscopy (AES); *X-ray spectroscopy*- principle and applications of X-ray fluorescence spectroscopy (XFS), X-ray absorption spectroscopy (XAS) and energy dispersive X-ray spectroscopy (EDS).

Group B

Infrared-Spectroscopy: Microwave Spectroscopy, stark Effect in microwave spectroscopy, linear harmonic oscillator, vibrational energies of diatomic molecules, zero point energy, force constant and bond strength, Morse potential energy diagram, vibration rotation spectroscopy, P, Q, R branches, break down of Born-Oppenheimer approximation, selection rules, overtones, hot bands, absorption by common functional groups, brief description of IR and FTIR instruments, application to metal-ligand vibrations/complex compounds, problems related to IR spectroscopy.

Electronic Spectroscopy: Different type of electronic transitions, Lambert's Beer's law, chromophores, auxochromes, solvent effect, red and blue shifts, Woodward's rule for conjugated cyclic and acyclic dienes and α, β–unsaturated carbonyl compounds, fluorescence and phosphorescence, spectra of transition metal complexes, charge transfer spectra, oscillator strength and intensity of the electronic transition, principle and applications of circular dichroism spectroscopy and time resolved spectroscopy problems related UV-Visible spectroscopy, absorption in aromatic compounds: substituted benzene, naphthalene and anthracene.

Scattering Spectroscopy: Principle and applications of traditional Raman spectroscopy, surface enhanced Raman spectroscopy (SERS), coherent anti-stoke's Raman spectroscopy (CARS).

Group C

Electron Spin Resonance Spectroscopy: Basic principle, factor affecting value, isotropic and anisotropic hyperfine coupling constant, g-Value, application to organic free radical, methyl free radical, naphthalene and benzene free radicals, CID NP, application of ESR in organic, inorganic and organometallic chemistry.

Mossbauer Spectroscopy: Theory, instrumentation, applications, isomeric shift, nuclear quadrupole coupling and hyperfine interaction, problems related to Mossbauer spectroscopy.

Mass Spectrometry: Instrumentation, mass spectra and molecular structure, fragmentation patterns in mass spectra, qualitative and quantitative analysis with mass spectrometry, measurement technique (El, Cl, FD and FAB), structure elucidation using mass Spectroscopy, GC-MS, laser mass spectrometry, electron spray ionization mass spectrometry, determination of molecular composition of organic compounds from mass spectra data.

Reference Books for CHE-613:

1. C. N. Banwell and E.M. McCash, *Fundamentals of Molecular Spectroscopy*, (4th Edition), Tata McGraw-Hill Publication Ltd., New Delhi, India (1995).

2. R. M. Silverstein, F. X. Webster, D. J. Kiemale and D. L. Bryce, *Spectrometric Identification of Organic Compounds* (8th Edition), John Wiley & Sons, Inc., New York, USA (2015).
3. R. Chang, *Basic Principles of Spectroscopy,* McGraw-Hill, New York (1971).
4. W. Kemp, *Organic Spectroscopy*, ELBS with Macmillan (1975).
5. Abragam & B. Bleaney, *Electron Paramagnetic Resonance of Transition Ions*, Oxford University, New York (1970).
6. S. M. Khopkar, *Basic Concepts of Analytical Chemistry*, (3rd Edition), New Age International Pvt. Ltd., New Delhi, India (2008).
7. P. Atkins and J. de Paula, *Atkins' Physical Chemistry,* (9th Edition), Oxford University Press, (2010).
8. J. Mendham, R. C. Denney, J. D Barnes, M. Thomas, B. Sivasankar, *Vogel's Quantitative Chemical Analysis*, (6th Edition), Pearson-India, (2011)
9. H. Kaur, *Instrumental Methods of Chemical Analysis*, (10th Edition), Pragati Prakashan, Meerut, India (2014).
10. V. K. Jha, *Theoretical Principles of Molecular Spectroscopy*, Kathmandu, Nepal (2011).

Elective Paper

Course Title: Biochemistry (Theory)
Course No.: CHE-614
Semester: Third (3rd)

Credit: Three (3) hrs.
Full Marks: 75
Pass marks: 37.5

Course Objectives:

- On completion of this course, the student should be able to explain the basic concepts of bioenergetics, metabolisms and biochemical techniques.

Course Contents:

Group A

Introduction: Definition, and scope of biochemistry.

Cell: Structural composition and functions of the prokaryotic cell, comparison of plants and animals cell and structural composition and metabolic functions of cell organelles, biological membranes, integral proteins of membrane, lipoproteins and trafficking through membrane, molecular logic of living organism.

Biomolecules: Structure, classification, physical and chemical properties in biochemical aspects, and function of proteins, carbohydrates, amino acids, lipids, nucleic acids, vitamins.

Enzymes: Definition, introduction, classifications and reactions, nomenclature, structure, isolation and purification and functions of enzymes, enzyme assay and activity, coenzymes and cofactors, isoenzymes, pro-enzymes, multienzyme complexes and tandom enzymes, regulation of enzyme activity: effects of pH, substrate, enzyme concentration, temperature, cofactor and additives, mechanism of enzyme action, enzyme specificity, active sites, covalent modification, kinetics of catalyzed reaction, Michaelis-Menten equation and its limitation, Briggs Haldane relationship. Inhibition of enzymes immobilized enzyme, applications of enzymes in clinical, foods, agriculture and environment.

Nucleic Acids: Structure and function of purine and pyrimidine nucleotides, codons and codon dictionary, type ribonucleic acids (RNA) and structures, structural composition of deoxyribonucleic acid (DNA), Watson and Crick model of DNA, Chargaff's rule. Biosynthesis of DNA (replication), biosynthesis of RNA

(transcription), and biosynthesis of protein (translation), sequencing and organization of genome, mutation, DNA drugs interaction.

Group B

Bioenergetics: Concept of standard free energy of reactions, relationship between equilibrium constant and standard free energy change, biological standard state and standard free energy change in coupled reactions, biological oxidation-reduction reactions and potentials, the importance of couple process in leaving things, high energy biomolecules, high energy phosphate compounds introduction, phosphate group transfer, free energy of hydrolysis of ATP and sugar phosphates.

Metabolism: Concept of metabolism, nutritional importance, digestion, absorption and transportation mechanism of activation of digestive enzymes.

Carbohydrate Metabolism: Carbohydrates source, chemistry, digestion, absorption, intestinal transport, glycolysis, HPM shunt, TCA cycle, glycogenolysis, glycogen synthesis, metabolism of sugar other than glucose, regulation of blood glucose level, gluconeogenesis, biosynthesis of disaccharides, glycoproteins, glyoxylate cycle, and metabolic regulation.

Amino acid Metabolism: Dynamic equilibrium of body protein, nutritional and metabolic importance of amino acids, catabolism of amino acids, metabolism of few individual amino acids, one- carbon fragment amino acids as biosynthetic precursor, urea cycle and metabolic diseases.

Lipid Metabolism: Concept of metabolism, nutritional importance, absorption, transportation, biosynthesis and degradation of simple and complex lipids, metabolism regulation, abnormalities in lipid metabolism.

Nucleotide Metabolism: Biosynthesis and degradation of purines and pyrimidines and their nucleotides, their interconversion and regulation, salvage pathway, regulation of biosynthesis of deoxyribonucleotides from ribonucleotide, abnormalities of purines and pyrimidines.

Group C

Microbial Biochemistry: Structural composition of gram positive and gram negative bacteria, structures and characteristics of bacterial protein toxin, basic concept of virion, prinos, lytic cycle, lysogeny and plasmid.

Biochemical Techniques: Principle and applications of centrifugation techniques, gel filtration chromatography, gel electrophoresis, optical rotatory dispersion, circular dichorism and X-ray diffraction techniques, gene transfer methods: electroporation and particle gun, MALDI-TOF technique, introduction of transgenic animals and plants.

Reference Books for CHE-614:

1. Lehninger, D. L. Nelson, and M. Cox Michael, *Lehninger Principle of Biochemistry*, (4th Edition), Macmillan Worth publisher, 2005.
2. Voet Donald, and Voet Judith G., *Fundamentals of Biochemistry*: *Life at the Molecular Level*, John Wiley & Sons, Inc., 2008.
3. Devlin, T. Wiley-Liss, *Textbook of Biochemistry with Clinical Correlation*, USA, 1997.
4. Jeremy M. Berg, John L. Tymoczko, Lubert Stryrer, *Biochemistry*, (5th Edition), W.H. Freeman and Company, 2002.
5. Robert K. Murray, Daryl K. Granner, Victor W. Rodwell Peter A. Mayes, *Harper's Illustrated Biochemistry*, Lange Medical Books/McGraw-Hill, 2003.

Elective Paper

Course Title: Analytical Chemistry (Theory) **Credit:** Three (3) hrs.
Course No.: CHE-615 **Full Marks:** 75
Semester: Third (3^{rd}) **Pass Marks:** 37.5

Course Objective:

- To provide advanced knowledge on chemical analysis and analytical techniques.

Course Contents:

Group A

Introduction: Analytical chemistry and chemical analysis, classification of analytical methods.

Selecting the Method: Factors to consider in choosing a method, performance criteria for methods to determine analyte in samples with the complex matrix, reason for incorrect analytical results, analytical validation.

Sampling Process: Types of sample, sampling plan, quality of sample, sub-sampling, sample registration and storage.

Measurement and Reporting: Good laboratory practices, calibration of measurements, record management, charting and reporting results.

Analytical Chemometrics: Propagation of measurement uncertainties (inaccuracy and imprecision). Useful statistical test: test of significance, the F test, the student 't' test, the chi-test, the correlation coefficient, confidence limit of the mean, comparison of two standard values, comparison of standard deviation with average deviation, comparison of mean with true values, significant figures, regression analysis (least square method for linear and non-linear plots), statistics of sampling and detection limit evaluation.

Karl-Fisher Titration: Stoichiometry of the reaction, preparation of the reagent, titration method, standardization of the reagent using water-in-methanol, determination of water in samples, interference and their elimination, application to quantitative analysis of some organic compounds-alcohols, carboxylic acids, acid anhydrides and carbonyl compounds.

Group B

Non-Aqueous Titrations: Acid-base titrations in non-aqueous solvents-classification of solvents, leveling and differentiating solvents, acidic and basic titrants, methods of titration, titrations in glacial acetic acid and ethylene diamine, applications of non-aqueous titrations.

Gravimetric Analysis: Formation and treatment of precipitates, co-precipitation, homogeneous precipitation, important precipitating agents and their significance in inorganic analysis.

Analytical Extraction Techniques: Aqueous extraction, solid phase extraction, solid phase micro-extraction, microwave assisted extraction, supercritical fluid extraction.

Group C

Hyphenated Techniques: Need for hyphenation, interfacing devices and applications of GC-MS, GC-IR, MS-MS, HPLC-MS, ICP-MS, ICP-OES.

Chemical Sensors: Principles, classification of chemical sensors, description of chemical sensors, optical sensors, calorimetric sensors, mass sensors, humidity sensors, biosensors

Reference Books for CHE-615:

1. D. A. Skoog, *Principles of Instrumental Analysis*, (3rd Edition), Saunders College Publishing, 1985.
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