Fourth Semester: Inorganic Chemistry

Subjects	Course Code	Credit Hours	Full Marks	Pass Marks
Bio-Inorganic Chemistry	CHE-651	4	100	50
Structure and Bonding in Complexes	CHE-652	4	100	50
Inorganic Chemistry Practical **OR** Inorganic Chemistry Dissertation	CHE-653 **OR** CHE-654	6 **OR** 6	150 **OR** 150	75 **OR** 75

Fourth Semester: Physical Chemistry

Subjects	Course Code	Credit Hours	Full Marks	Pass Marks
Advanced Electrochemistry and Corrosion Science	CHE-655	4	100	50
Molecular Spectroscopy	CHE-656	4	100	50
Physical Chemistry Practical **OR** Physical Chemistry Dissertation	CHE-657 **OR** CHE-658	6 **OR** 6	150 **OR** 150	75 **OR** 75

Fourth Semester: Organic Chemistry

Subjects	Course Code	Credit Hours	Full Marks	Pass Marks
Organic Stereochemistry	CHE-659	4	100	50
Organic Spectroscopy	CHE-660	4	100	50
Organic Chemistry Practical **OR** Organic Chemistry Dissertation	CHE-661 **OR** CHE-662	6 **OR** 6	150 **OR** 150	75 **OR** 75

Inorganic Chemistry

Course Title: Bio-Inorganic Chemistry (Theory) **Credit:** Four (4) hrs.
Course No.: CHE-651 **Full Marks:** 100
Semester: Fourth (4^{th}) **Pass Marks:** 50

Course Objective:

- To acquaint the students with basic principles of bio-inorganic chemistry.

Course Contents:

Group A

Bio-Inorganic Chemistry:

Metal Complexes as Oxygen Carriers: Hemoglobin and myoglobin, non-porphyrin oxygen carriers, hemerythrin and hemocyanin and model compounds.

Biochemistry of Iron Metal Complexes: Ferritin, transferin, siderophores for storage and transfer and model compounds.

Group B

Electron Carrier Proteins: Ferredoxins and rubredoxins, blue copper proteins, cytochrome and model compounds.

Photosynthesis: Chlorophyll and the photosynthetic reaction center and model compounds.

Group C

Metalloenzymes: Carboxypeptidase, carbonic anhydrase oxidases, vitamin B_{12} and the B_{12} coenzymes, nitrogenases and model compounds.

Dioxygen Involved in Enzymes: Tyrosinase, methane monooxygenase, dioxygenase, ribonucleotide reductase and model compounds.

Group D

Metal Based Drugs: Anticancer activity of Sn, Ru, Pt, Ga, Ti complexes, medicinal value of Au complexes, other metal compounds as drug.

Sensors.

Transport of metal ions in biological Systems, ion pumps, ionophores, nucleic acid and metal interactions.

Reference Books for CHE-651:

1. Bertini, H.B.Gray, S.J. Lippard and J.S. Valentine EDs., *Bio-Inorganic Chemistry*,University Science Books, Mill Valley, CA, 1994.
2. S.J. Lippard and J.M. Berg, *Principles of Bioinorganic Chemistry*, University Science Books, Mill Valley CA, 1994.
3. J.R.F. da Saliva, R.J.P. Williams, *The Biological Chemistry of the Elements - The Inorganic Chemistry of Life*, Clarendon Press, Oxford, 1991.
4. A.K. Bhagi and G.R. Chatwal, *Bioinorganic and Supramolecular Chemistry*, Himalaya Publishing House Pvt. Ltd., Delhi, 2014.

Inorganic Chemistry

Course Title: Structure and Bonding in Complexes (Theory) **Credit:** Four (4) hrs.
Course No.: CHE-652 **Full Marks:** 100
Semester: Fourth (4^{th}) **Pass Marks:** 50

Course Objectives:

- To provide them with knowledge on theories of bonding and structures of inorganic compounds.

Course Contents:

Group A

Ligand Field Spectra of Octahedral Complexes: Energy states from spectral terms, Selection rules, La Porte's rule, spin selection rule, band intensities, factors affecting bandwidth, effect of temperature on absorption spectra, splitting diagrams: splitting for d^1, d^9, and high spin d^4 and d^6, splitting for d^2, d^3, d^8 and high spin d^7, high spin d^5, non-crossing rule, Tanabe-Sugano diagrams, correlation diagrams, Racah

parameter, energy level calculations, spectra of d^1-d^6 ions, spectra of second and third row transition elements, lowering of symmetry, effects of lowering symmetry, charge transfer bands.

Group B

Molecular Orbital Description of Bonding: Bonding in octahedral complexes, bonding in tetrahedral complexes, quantitative calculation of 10Dq, effects of π bonding, Elementary group theoretical treatment for sigma bonding and π bonding in octahedral complexes, comparison of the different approaches to bonding in co-ordination compounds.

Abnormal Valency: Unusual oxidation states: Metal ions in low and high oxidation states, Factors affecting the stabilization of abnormal valencies, Preparation of complexes of metal in zerovalent state, stabilization of oxidation states and π bonding, stabilization of low oxidation states through coordination, Ligands which stabilize both low and high valent states.

Group C

Magnetic Properties of Complex Ions: The theory of magnetic susceptibility, the magnetic properties of free ions, quenching of orbital angular momentum by ligand fields, the magnetic properties of A and E terms, the magnetic properties of T terms, the magnetic properties of complexes with A and E ground terms, the magnetic properties of complexes with T ground term, spin-free-spin-paired equilibria.

Group D

Important Complexes of Gr VIIB, Gr VIII and Actinide Elements:

Group Discussion: Chemistry of Gr. VIIB (7) Technetium and Rhenium:

Oxidation states and stereochemistry: Important compounds: oxides and sulphides, halides, multiple bonded dirhenium and ditechnitium compounds, oxo compounds and complexes.

Chemistry of Gr. VIII Platinum Group Metals (Ru, Os, Rh, Ir, Pd, Pt):

Review on occurrence and general remarks and extraction on the chemistry of platinum metals. Important compounds: Ruthenium and Osmium Group VIII (8): Oxidation state, coordination number and geometry, oxo-compounds of ruthenium (Ru) and osmium(Os), halide complexes, complexes of nitrogen donor ligands, nitric oxide complexes, tertiary phosphine and related complexes, lower oxidation states, Grubb's catalyst.

Rhodium and Iridium Group VIII (9): General remarks: Stereochemistry, oxidation states, coordination number and stereochemistry, complexes of Rh (I) and Ir (I), complexes of Rh (II) and Ir (II), complexes of Rh (III) and Ir (III), complexes of Rh (IV) and Ir (IV), palladium and platinum Group VIII (10): oxidation state, coordination number and stereochemistry, complexes of Pd (II) and Pt (II), complexes of Pd (IV) and Pt (IV), mixed valence and linear chain compounds, complexes of Pd (III) and Pt (III), complexes of Pd and Pt in low oxidation state.

Actinide Element: Occurrence, separation and general properties, general chemistry of the actinides: occurrence, survey of oxidation state, actinide ions in aqueous solution, complexes and stereochemistry of actinide elements, organometallic chemistry of actinide elements, chemistry of individual elements, uranium and thorium, the transuranium elements Np, Pu and Am, the trans-americium elements, the super heavy elements.

Reference Books for CHE-652:

1. A.B.P. Lever, *Inorganic Electronic Spectroscopy*, (2^{nd} Edition) Elsevier, Amsterdam, 1984.
2. B.N. Figgis, *Introduction to Ligand Fields*, Interscience Publishers, 1966.
3. J.K. Burdett, *Molecular Shapes;* Wiley-Interscience, New York, 1980.
4. J. Lewis and R.G. Wilkins, *Modern Co-ordination Chemistry*, Interscience Publishers.
5. D. Katakis and G. Gordon, *Mechanism of Inorganic Reactions*, John Wiley and Sons, New York, 1987.
6. C. H. Langsford and H.B. Gray, *Ligand Substitution Processes*, Benjamin Commings, 1966.

7. F. A. Cotton, G. Wilkinson, C.A. Murillo and Manfred Bochmann, *Advanced Inorganic Chemistry*, (6^{th} Edition), John Wiley and Sons, 1999.
8. Satya Prakash, *Advanced Chemistry of Rare Elements,* (Revised Edition) S.Chand and Company Ltd. 2013.
9. K.W. Bagnall, *The Actinide Elements,* American Elsevier, Amsterdam, 1972.
10. Ed. M. M. Edelstein, *Actinides in Perspective*, Pergmon Press, New York, 1982.
11. J. J. Katz, G.T. Seaborg and L.R. Morss, *The Chemistry of the Actinide Elements, 2nd Ed.,* Chapman and Hall, 1986.
12. M. A. K. Lodhi, *Superheavy Elements*, Permagon Press, New York, 1976.
13. C. Keller, *The Chemistry of Transuranium Elements*, Springer Verlag, 1971.
14. Robert H. Grubbs, Olefin Metathesis Catalysts for the Preparation of Molecules and Materials, Nobel Lecture, December 8, 2005
15. Kettler, Peter B., *Platinum Group Metals in Catalysis: Fabrication of Catalysts and Catalyst Precursors*, Organic Process Research & Development, *7*, 342-354.
16. C. J. Ballhausen, *Introduction to Ligand Field Theory*, McGraw Hill, 1962.

Inorganic Chemistry

Course Title: Inorganic Chemistry Practical
Course No.: Che-653
Semester: Fourth (4^{th})
Credit: Six (6) hrs.
Full Marks: 150
Pass Marks: 75

Course Objectives:

- To acquaint the students with various techniques of qualitative and quantitative analysis.
- To acquaint the students with techniques for the preparation, characterization and estimation of inorganic complexes.
- To help the students in developing skills for planning analytical works.
- To familiarize them with making use of some instruments.

Course Contents:

Salt analysis:

1. Qualitative analysis of inorganic salt mixture containing 8 radicals including rare elements and interfering radicals by semi-micro method.

Instrumental

1. Determination of equilibrium constant.
2. Estimation of Na, K and calcium by flame photometry.
3. Estimation of iron in a sample of tomato juice spectrophotometrically.
4. Qualitative analysis of inorganic cations of Gr. I, II, III and IV and anions by paper chromatography.
5. Separation of metal cations by column chromatography.
6. Spectrophotometric determination of phosphate by molybdenum blue method.
7. Spectrophotometric determination of arsenic by molybdenum blue method.

Gravimetric Analysis:

1. Estimation of different metals present in the given sample of brass gravimetrically.
2. Determination of nickel in nickel steel.
3. Estimation of calcium and magnesium in dolomite.

4. Analysis of Portland cement

Analysis of any four alloys.

Preparation:

1. Preparation and aquation of $Co(NH_3)_5Cl^{2+}$
2. Extraction of chlorophyll from plant leaves.
3. Synthesis and study of an oxygen-carrying cobalt complex.
4. Preparation of manganese dioxide nano-particles.
5. Preparation of a chemical fertilizer.

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

Reference Books for CHE-653:

1. M.R. Pokhrel, P.N. Yadav and S. Shrestha, *Advanced Practical Inorganic Chemistry* for M.Sc., (2^{nd} Edition), Kshitiz Publication, 2017.
2. A.I. Vogel, *Qualitative Analysis*; E.L.B.S., 1994.
3. Palmer, *Experimental Inorganic Chemistry*, Cambridge University Press, UK, 1954.
4. Angelici, *Synthesis and Technique in Inorganic Chemistry*; W.B. Sounders Co. (Sounders Golden Series), Philadelphia, 1991.

Inorganic Chemistry

Course Title: Inorganic Chemistry Dissertation
Course No.: CHE-654
Semester: Fourth (4^{th})

Credit: Six (6) hrs.
Full Marks: 150
Pass Marks: 75

Course Objectives:

- To make the students familiar with research works in inorganic chemistry and related fields.
- To make the students able to do independent research work.

Course Contents: Research work on a topics provided by the supervisor.

General Guidelines for M. Sc. Dissertation in Chemistry: The student will work on a research problem and will generate results by independently conducting inorganic chemistry experiments and analyzing the data. The student is expected to find out some novel finding in his/her research work and write a dissertation on a format prepared by the Central Department of Chemistry, Tribhuvan University. The student will defend his/her finding in an open oral examination.

Physical Chemistry

Course Title: Advanced Electrochemistry and Corrosion Science (Theory)
Course No.: CHE-655
Semester: Fourth (4^{th})

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

Course Objectives:

- ❖ To give the knowledge of advanced electrochemistry with emphasis on modern electrochemical techniques.
- ❖ Explore the knowledge of metallic corrosion and its control methods.

Course Contents:

Group A

Electrode Kinetics: Introduction; charge transfer and its chemical and electrical implications; charge transfer under zero field; electron transfer under an interfacial field, equilibrium exchange current; non-equilibrium drift current; overpotential; basic electrodic equation: Butler-Volmer equation, some general and special cases; low and high field (Tafel plot and its applications and limitations) approximations, physical meaning of symmetry factor; polarizable and non-polarizable interfaces; Nernst equation; multistep electrode reactions; rate determining step and energy barrier for multiple step reaction; order of electrodic reaction; determination of reaction mechanism of iron deposition and dissolution; mass transfer to electrode surface; microscopic theories of charge transfer -Marcus microscopic model.

Group B

Technologically Interested Electrochemical Processes: *Semiconductor electrode:* Current-potential curves at semiconductor electrodes; photo-effects at semiconductor electrodes, photo-electrochemical cells: some photo-electrochemical phenomenon (splitting of water, reduction of CO_2, waste removal and surface photo-catalytic process); prospects of photo-electrochemical solar cell; *Electrochemical energy conversion:* Introduction; present situation of energy consumption and global concern on environment; concept of hydrogen energy and hydrogen economy; efficiency of an electrochemical energy convertor, condition for maximum efficiency, fuel cells (types, details on polymer electrolyte, direct methanol fuel and solid oxide fuel cells); *Electrochemical energy storage:* Introduction, capacity of battery: energy density and power density, details on lead-acid, zinc-manganese alkaline, metal-hydride and Li-ion batteries, charge-discharge of a battery, Ragone plot, super-capacitor (introduction, types and prospects); *Electro-catalysis:* introduction, common types of electro-catalyst, electro-catalyst for hydrogen evolution, oxygen reduction and methanol oxidation reactions; design of electro-catalysts; *Electro-deposition:* introduction, various steps in electro-deposition, deposition to crystallization, effect of overpotential.

Group C

Corrosion Science: Review lecture of definition, importance and types of corrosion; *electrochemical mechanisms of corrosion*: electrochemistry of corrosion cell, electrochemical theory of corrosion; heterogeneous; homogeneous and mixed-potential theories; corrosion current and corrosion potential; *corrosion tendency of metallic substances*: potential-pH diagrams for water and M/H_2O systems; applications of potential-pH diagram for corrosion and its control with reference to Fe/H_2O systems; steel corrosion in different corrosive media reference with the potential-pH diagram; advantages & limitations of the potential-pH diagram; *corrosion kinetics:* at equilibrium and under polarization; Evans diagram and corrosion kinetics, corrosion estimation methods.

Group D:

Corrosion Control and Passivation: *General methods of corrosion control*: environmental factors; design of corrosion-resistant metallic materials; materials selection; corrosion coatings with reference metallic and non-metallic coatings*; corrosion inhibitor*: types; mechanism of corrosion inhibitor*; cathodic protection*: principles; advantages; limitations and comparison of impressed-current and sacrificial anode techniques*; anodic protection*: principle; advantages & limitations.

Passivation of metallic materials: Definition; polarization & passivity; stability & Flade potential; factors for passivation; *theories of passivation*: oxide-film formation; adsorption and other theories.

Electrode Techniques for Corrosion Kinetics: Introduction; potential step and potential sweep methods, controlled-current method (potential-time curves); hydrodynamic electrodes: introduction; principle, advantages and limitations of rotating disk and rotating ring electrodes.

Reference Books for CHE-655:

1. J. O'M. Bockris and A. K. N. Reddy, *Modern Electrochemistry*, Vol. 1, (2nd Edition), Plenum Publ. Corp., New York, USA, 1998.
2. J. O'M. Bockris, A. K. N. Reddy and M. Gamboa-Aldeco, *Modern Electrochemistry: Fundamentals of Electrodics*, Vol. 2A, (2nd Edition), Kluwer/Plenum Publ., New York, USA, 2000.
3. J. O'M. Bockris, A. K. N. Reddy and M. Gamboa-Aldeco, *Modern Electrochemistry*: *Electrodics in Chemistry, Engineering, Biology and Environmental Science*, Vol. 2B, (2nd Edition), Kluwer/Plenum Publ., New York, USA, 2000.
4. R. W. Revie and H. H. Uhlig, *Corrosion and Corrosion Control: An introduction to Corrosion Science and Engineering*, (4th Edition), John Wiley & Sons Inc., New York, USA, 2008.
5. J. Bhattarai, *Frontiers of Corrosion Science*, (1st Edition), Khitiz Publ., Kathmandu, Nepal, 2010.
6. P. R. Roberge, *Corrosion Engineering: Principles and Practice*, McGraw-Hill co., Inc, New York, USA, 2008.
7. D. Talbot and J. Talbot, *Corrosion Science and Technology*, CRC Press LLC, New York, USA, 1997.
8. A. J. Bard and L. R. Faulkner, *Electrochemical Methods: Fundamentals and Applications*, (2nd Edition), John Wiley & Sons Inc., New York, USA, 2001.

Physical Chemistry

Course Title: Molecular Spectroscopy (Theory) **Credit:** Four (4) hrs.
Course No.: CHE-656 **Full Mark:** 100
Semester: Forth (4th) **Pass Mark:** 50

Course Objectives:

- To understand the principles of molecular spectroscopy
- To develop skills in quantitative analysis of spectral data

Course Contents:

Group A

Rotational and Vibrational Spectroscopy: Review on rotational and vibrational spectra; *Rotational spectra*: quantum mechanical results on rigid rotator; Stark effect; rotational spectra of symmetric top and asymmetric top molecules; non-rigid rotator, energy levels and spectrum; *Vibrational spectra*: vibrational energies of diatomic molecules, zero point energy, force constant and bond length, calculation of bond lengths, dissociation energies, anharmonic oscillator, energy levels diatomic vibrating rotator, vibration of polyatomic molecules, overtones and hot bonds, P, Q and R branches, application of vibration spectra in elucidation of molecular structure from vibrational frequencies.

Group B

Raman Spectroscopy: Techniques and instrumentation; pure rotational and Raman spectra: symmetric and asymmetric top molecules; vibrational Raman spectra: Raman activity of vibration; overtone and combination vibrations; rotational fine structure; vibration of spherical top molecules; structure determination by Raman and infrared spectroscopy.

Electronic Spectroscopy: Observed intensity distribution in absorption; wave mechanical formulation of Franck-Condon principle; electronic transitions; singlet and triplet states; fluorescence and phosphorescence; dissociation and pre-dissociation; calculation of electronic transitions of polyenes using free electron model (particle in a box).

Lasers, Laser Spectroscopy and Photochemistry: Population inversion and three level systems, components of laser, high resolution laser spectroscopy, pulsed laser and dynamics of photochemical processes.

Group C

Nuclear Magnetic Resonance Spectroscopy: Theory of NMR spectroscopy; energies of nuclei in magnetic fields; NMR-spectrometer; relaxation process in NMR; chemical shift and affecting factors; spin-spin coupling; coupling constant and affecting factors; nuclear overhauser effect (NOE); Fourier transform NMR and its advantages; NMR spectra of simple molecules.

Multinuclear Solid-State NMR Spectroscopy: *^{29}Si NMR spectroscopy*: broadening, relaxation and structural effects; ^{29}Si NMR chemical shifts in Si-O compounds and its applications for silicate glasses, gels and cements identification; *^{27}Al NMR spectroscopy*: introduction, chemical shifts in ^{27}Al NMR spectra and its applications for aluminium oxides, amorphous aluminium compounds and cement identification.

Group D

Electron Spin Resonance Spectroscopy: Introduction; basic principles and magnetic interactions; instrumentation and signal generation; quantitative analysis; modern ESR techniques: electron nuclear double resonance (ENDOR) and pulsed ESR; applications of ESR in molecular sieve science.

Mössbauer Spectroscopy: Introduction; principle; Lamb Mössbauer factor; Mössbauer nuclides; parameters for Mössbauer spectra: isomer shift, quadrupole shifting, magnetic splitting and time-dependent effects, relaxation and dynamics; some applications of Mössbauer spectroscopy.

Reference Books for CHE-656:

1. C. N. Banwell and E.M. McCash, *Fundamentals of Molecular Spectroscopy*, (4th Edition), Tata McGraw-Hill Publication Ltd., New Delhi, India, 1995.
2. P. Atkins and J. de Paula, *Atkins' Physical Chemistry*, (10th Edition), Indian edition, Oxford University Press, India, 2014.
3. D. A. McQuarrie and J. D. Simon, *Physical Chemistry: a Molecular Approach*, Viva Student Edition, Viva Books Pvt. Ltd., New Delhi, India, 2011.
4. K. J. D. MacKenzie and M. E. Smith, *Multinuclear Solid-State NMR of Inorganic Materials* (Ed. R. W. Cahn), Pergamon; an imprint of Elsevier Science Ltd., Amsterdam, The Netherlands, 2002.
5. G. Hertzberg, *Molecular Structure and Molecular Spectra*: *Vol. 1 Spectra of Diatomic Molecules*, (2nd Edition), Van Nostrand, Reinhold, New York, USA, 1950.
6. B. M. Weckhuysen, R. Heidler and R. A. Schoonheydt, *Electron Spin Resonance Spectroscopy, Molecular Sieves*, 4, 295-335, 2004.
7. V. K. Jha, *Theoretical Principles of Molecular Spectroscopy*, Kathmandu, Nepal, 2011.
8. P. S. Sindhu, *Molecular Spectroscopy*, Tata McGrow-Hill Publication Ltd., New Delhi, India, 1985.
9. 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.

10. D. P. E. Dickson and F. J. Berry, Mössbauer Spectroscopy, Cambridge University Press, Cambridge, London, 1986.
11. B. K. Sharma, *Spectroscopy*, Krishna Prakashan Media Pvt. Ltd., Meerut, India (2013).
12. H. Kaur, *Instrumental Methods of Chemical Analysis*, (10^{th} Edition), Pragati Prakashan, Meerut, India, 2014.

Physical Chemistry

Course Title: Physical Chemistry Practical
Course No.: CHE-657
Semester: Forth (4^{th})
Credit: Six (6) hrs.
Full Mark: 150
Pass Mark: 75

Course Objective:

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

Course Contents:

Electrochemistry

1. Experiments involving corrosion measurement and corrosion inhibition.
2. Experiments involving controlled potential and controlled current measurement method.
3. Determination of different metal ions by polarographic method.
4. Determination of decomposition and half wave potentials of different metal ions.
5. Determination of the effects of ionic strength on the solubility of $CaSO_4$ and so thermodynamic solubility product and mean ionic activity.

Chemical Kinetics

6. Kinetic study of the autocatalytic reaction between MnO_4^- and $C_2O_4^{2-}$ ions catalyzed by Mn^{2+} ions.
7. Determination of the activation energy for the reaction between ethyl acetate and sodium hydroxide using conductance measurement.
8. Kinetic study of inversion of sugar by polarimeter.

Colorimetry /Spectrophotometry

9. Kinetic study for oxidation of alcohol by dichromate by colorimetric method.
10. Determination of iron in tomato by spectrophotometric method.

Miscellaneous

11. Determination of cation exchange capacity (CEC) of natural clays, silica gel, activated charcoal etc.
12. Determination of the physical and sintering properties of locally available ceramic tiles and bricks.
13. Determination of sodium and potassium in tomato or oral hydration powder (Jeevan Jal).
14. Separation by column chromatography and ion exchange chromatography.
15. Experiments involving the analysis of FTIR spectra and X-ray diffraction (XRD).

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

Reference Books for CHEM-657:

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*: (9th 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.

Physical Chemistry

Course Title: Physical Chemistry Dissertation
Course No.: CHE-658
Semester: Forth (4th)
Credit: Six (6) hrs.
Full Mark: 150
Pass Mark: 75

Course Objectives:

- To make the students familiar with research works in Physical Chemistry and related fields.
- To make the students able to do independent research work.

Course Contents: Research work on a topics provided by the supervisor.

General Guidelines for M. Sc. Dissertation in Chemistry: The students will work on a research problem and will generate results by independently conducting Physical Chemistry experiments and analyzing the data. The student is expected to find out some novel finding in his/her research work and write a dissertation on a format prepared by the Central Department of Chemistry, Tribhuvan University. The student will defend his/her finding in an open oral examination.

Organic Chemistry

Course Title: Organic Stereochemistry (Theory)
Course No.: CHE-659
Semester: Fourth (4th)
Credit: Four (4) hrs.
Full Marks: 100
Pass Marks: 50

Course Objective:

- To provide students a panoramic view of the stereochemistry of various organic compounds.

Course Contents:

Group A

Configuration: Relative and absolute configuration, determination of relative configuration of saturated aliphatic compounds (chemical interconversion not affecting bonds to the stereogenic atom, correlation via compounds with chiral centers of two types, chemical correlations affecting bonds to a chiral atom in a known way, correlation by stereoselective synthesis of known stereochemical course. Determination of configuration of *cis-trans* isomers (chemical methods, physical methods), interconversion of *cis-trans* isomers (photochemical isomerization, directed *cis- trans*interconversion.

Conformation of Acyclic Molecules: conformation of ethane, butane and other simple saturated acyclic molecules, conformation of unsaturated acyclic compounds, physical and spectral properties of diastereomers and conformers (dipole moment, b.p., refractive index, density, IR spectra, NMR spectra), conformation and reactivity.

Group B

Configuration and Conformation of Cyclic Molecules: stereoisomerism and configurational nomenclature of ring compounds (symmetry based method), Stability of cyclic molecules, strain, ease of cyclization as a function of ring size, ease of ring closure as a function of the ring atoms and substituents, conformational aspects of the chemistry of six membered ring compounds, mono, di- and polysubstitutedcyclohexanes, The Thorpe – Ingold Effect Balwin's Rules, conformation and reactivity in cyclohexanes, chemistry of three and four membered rings, rings larger than six membered, concept of I-strain.

Stereochemistry of Fused Rings: Hydrindanes, decalin, perhydrophanenthrene and perhydroanthracenes, bridged rings, Bredt's rule and bridge head alkenes, cryptands, crown ether, podands and spherands, paddlanes and propellanes, atenanes, rotanances, knots and Mőbius strips, synthesis of cubane, adamantane, tetrahedrane, dodecahedrane and Buckminster fullerene.

Group C

Stereoselective Synthesis: diastereoselective synthesis of achiral compounds (cyclanes, stereocontrolled synthesis of E-alkene derivative via alanes and (E,E) farnesol convergent synthesis), diastereoselectivesythesis based on chiral substrates- (addition of nucleophile- Felkin transition states for addition of a nucleophile to cyclohexanone, eletrophilic reactions of alkenes- alkylation of a cyclohexylideneenolate anion, the aldol reaction, catalytic hydrogenation free radical addition), enantioselective synthesis (chiral organometal complexes, catalysis by chiral bases, enzyme based processes, enantioselectivedeprotonation of cyclohexanone derivatives) enantioconvergent synthesis via the Claisen rearrangement.

Group D

Chiroptical Properties: Optical activity, anisotropic refraction (origin, theory, optical rotatory dispersion), circular dichrosim, anisotropic absorption, application of optical rotatory dispersion and circular dichroism (determination of configuration and conformation), saturated ketones (the octant rule)

Chiralty in Molecules Devoid of Chiral Centers: Introduction and nomenclature, allenes, synthesis of optically active allenes, determination of configuration, cyclic allenes, alkylidenecyclohexanes, spiranes, biphenyl (atropisomerism), biphemyls and other atropisomers of the sp^2 - sp^2 single bond type, configuration of biphenyls and binaphthyls, molecular propellers, molecules with planar chirality (cyclophanes and annulenes).

Reference Books for CHE-659:

1. E. L. Eliel, S. H. Wilen and L. N. Mander, *Stereochemistry of Organic Compound*, John Wiley & Sons, Inc., 1994.
2. E. L. Eliel, *Stereochemistry of Carbon Compounds*, McGraw Hill Book Comp. Inc, 1975.
3. K. Mislow, *Introduction to Stereochemistry*, W.A. Benjamin Inc, 1966.
4. M. Nógrădi, *Stereoselective Synthesis*, VCH Publishers, 1995.
5. I. L. Finar, *Organic Chemistry*, vol I and II; ELBS 1975.
6. K. R. Palak, *Stereochemistry*, Pairavi Prakashan, Kathmandu, Nepal, 2017.

Organic Chemistry

Course Title: Organic Spectroscopy (Theory) **Credit:** Four (4) hrs.
Course No.: CHE-660 **Full Marks:** 100
Semester: Fourth (4^{th}) **Pass marks:** 50

Course Objective:

- To provide students a panoramic view of the spectroscopic techniques in structure elucidation of various organic compounds.

Course Contents:

Group A

Ultraviolet Spectroscopy: Introduction, theory, sample handling, characteristic adsorption of organic compounds, compound containing only σ electron, saturated compound containing n electrons and compound containing π electron, chromophores, auxochromes, bathochromic shift and hypsochromic shift, rules for predicting the position of absorption of homo- and heteroannuler systems, problems.

Infrared Spectroscopy: Introduction, theory, coupling interaction and hydrogen bonding, instrumentation, dispersion IRspectrometer, fourier transform infrared spectrometer, sample handling, interpretation of spectra, characteristic group adsorption of organic molecules, normal alkane, branch chain alkane, cyclic alkanes, cyclic alkanes, alkenes, alkynes, aromatic hydrocarbon, alchohol, phenol, ether, epoxide, peroxide, ketones, aldhydes, carboxylic acids, ester, acid halides, carboxylic acid, amide, amine etc, problems.

Group B

NMR Spectroscopy (Nuclear Magnetic Resonance Spectroscopy):

^{1}H-NMR: Introduction, CWNMR spectroscopy, relaxation (longitudinal and transverse), pulse FT^{1}H-NMR spectrometry, and rotatory frame of reference, instrumentation, sample handling, chemical shift, simple spin coupling, protons on heteroatoms, proton on an oxygen atom, nitrogen and sulfur, coupling of protons to other nuclei, chemical shift equivalence and magnetic equivalence, determination of chemical shift equivalence by interchange through symmetry operation, tagging and interconversion of structure, magnetic equivalence, AMX, ABX and ABC systems with the coupling constants, strongly and weakly coupled spin systems, effect of a chiral center, nuclear Overhauser effect, shift reagents and problems.

^{13}C-NMR spectroscopy: Introduction, peak assignments, off resonance decoupling, chemical shifts of alkane, alkene, alkyne, aromatic compound, hetero aromatic compound, alcohol, ether, halide, amide etc., chemical shift equivalence, spin coupling (^{1}H^{13}C J values), DEPT spectrum, and problems.

Group C

New Dimensions in NMR: Introduction, ^{1}H-^{1}H connectivity, Homo J-resolved ^{1}H-^{1}H spectroscopy, correlated spectroscopy (COSY), ^{1}H-^{13} connectivity, J- resolved ^{1}H^{13}C spectroscopy (HET 2DJ), heteronuclear chemical shift correlation (HETCOR), ^{13}C-^{13}C connectivity, NOE difference spectrum (1-D) and the NOESY (nuclear Overhauser and exchange spectroscopy) (2-D), ROESY, HMBC, HMQC, and problems.

Group D

Mass Spectrometry: Introduction, mass spectrum, instrumentation, magnetic field only, double focusing (electrostatic and magnetic field), quadrupole mass filter, quadrupole ion storage, time of flight, and MS/MS (Tandem Mass Spectrometry), determination of molecular formula, unit mass molecular ion and isotope peaks, high resolution molecular ion, recognition of molecular ion peak, other useful ionization techniques (CI, FD, FAB, ESI, MALDI), use of molecular formula and index of hydrogen deficiency, fragmentation, hemolytic cleavage and heterolytic cleavage, rearrangements, hydrogen transfer, McLafferty and random,

mass spectra of some chemical classes (hydrocarbon, hydroxy compounds, ether, ketone, aldehyde, amine, amide, halogen compound etc.), problem solving.

Reference Books for CHE-660:

1. R. M. Silverstien, F. X. Webster, *Spectrometric Identification of Organic Compounds* (6th Edition), John Wiley & Sons, Inc., 1998.
2. R. M. Silverstien, G. C. Bassler and T. C. Morrill, *Spectrometric Identification of Organic Compounds* (5th Edition), John Wiley & Sons, Inc., 1991.
3. R. M. Silverstien, F. X. Webster, D. J. Kiemle, D. L. Bryce, *Spectrometric Identification of Organic Compounds* (8th Edition), John Wiley & Sons, Inc., 2015.
4. J. R. Dyer, *Application of Absorption Spectroscopy of Organic Compounds*, Prentice Hall, Inc. 1965.
5. Y. R. Sharma, *Elementary Organic Spectroscopy*, S. Chand and Company, New Delhi, 2013.
6. Atta Ur Rahmann, *Nuclear Magnetic Resonance*, *Basic Principles*, *Springe Verlag*, YK, 1986.

Organic Chemistry

Course Title: Organic Chemistry Practical
Course No.: CHE-661
Semester: Fourth (4th)

Credit: Six (6) hrs.
Full Marks: 150
Pass Marks: 75

Course Objective:

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

Course Contents:

1. Synthesis of organic compounds involving three steps and their characterization by spectroscopic and chemical techniques.
2. Determination of quality of oil.
3. Isolation of mucic acid from milk.
4. Determination of vitamin C in fruit juices.
5. Determination of amino group.
6. Determination of protein in milk by titration method.
7. Determination of hydroxyl group.
8. Determination of nitrogen by Kjeldahl's method.
9. Determination of sulphur by gravimetric method.
10. Determination of percentage purity of sugar.
11. An experiment on vacuum distillation of organic compound.
12. An experiment on semi micro techniques.
13. Purification of water through a fabricated charcoal column.

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

Reference Books for CHE-661:

1. B. B. Dey, M. V. Sitaraman and T. R. Govindachari, *Laboratory Manual of Organic Chemistry* (3rd Edition), S. Vishwanathan Publisher.

2. N. K. Vishnoi, *Advanced Practical Organic Chemistry* (2nd Edition), Vikas Publishing Pvt. Ltd, 1996.
3. A. I. Vogel, *A Text Book of Practical Organic Chemistry* (5th Edition), Longman, 1989.
4. 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.
5. J. B. Harborn*et al.*, Phytochemical Methods (2nd Edition), Chapman Hall, London, 1984.
6. P. J. Houghton, A. Rahaman, *A Laboratory Manual for Fractionation of Natural Extracts*, Chapman Hall, London, 1998.

Organic Chemistry

Course Title: Organic Chemistry Dissertation
Course No.: CHE-662
Semester: Forth (4th)

Credit: Six (6) hrs.
Full Mark: 150
Pass Mark: 75

Course Objectives:

- To make the students familiar with research works in Organic Chemistry and related fields.
- To make the students able to do independent research work.

Course Contents: Research work on a topics provided by the supervisor.

General Guidelines for M. Sc. Dissertation in Chemistry: The students will work on a research problem and will generate results by independently conducting Organic Chemistry experiments and analyzing the data. The student is expected to find out some novel finding in his/her research work and write a dissertation on a format prepared by the Central Department of Chemistry, Tribhuvan University. The student will defend his/her finding in an open oral examination.