

Institute of Science and Technology

Master of Science in Chemistry

M. Sc. Chemistry (Semester System)

Curriculum

2017 (2074)



Tribhuvan University

Nepal

Master of Science in Chemistry

M. Sc. Chemistry Curriculum

Effective from 2017 (2074)

Institute of Science and Technology

Tribhuvan University

Kathmandu, Nepal

Introduction:

Four year Bachelor level education (previously three years) has been introduced in Tribhuvan University in order to bring the standard of education on a par with international standard. The readjustment made in this way has therefore necessitated modifying and revising the present syllabus for the Master's degree programme.

Objectives:

The main objectives of the course are:

- * To modernize and upgrade the quality of Master level program in Chemistry so that the academic level comes up to the existing international standard.
- * To make the students capable of initiating and understanding scientific research work in chemistry by providing them with an in-depth knowledge of chemistry in the areas of its specialized branches.
- * To make the academic program more relevant and pragmatic according to the professional needs and to achieving national objectives.
- * To make the students capable of planning and pursuing independent study and research in chemistry.
- * To familiarize the students with the tools and techniques used in chemistry and in related fields.
- * To provide knowledge in interdisciplinary subjects related to chemistry.

Eligibility or Admission:

The candidate who have passed B. Sc. Degree with major in chemistry from Tribhuvan University or have received equivalent degree with chemistry as major from another university recognized by Tribhuvan University shall be considered eligible to apply for admission to M. Sc. Chemistry.

Admission Criteria:

An applicant seeking admission to M. Sc. Chemistry must appear in an Entrance Examination of two hours duration conducted by the Institute of Science and Technology, Central Department of Chemistry, Tribhuvan University. The applicant who fails to appear in the Entrance Examination or to obtain a minimum qualifying score will not be given admission. A merit list of the qualified applicants will be prepared on the basis of marks obtained by them in the entrance examination. Admission of the students will be based strictly on the merit list and on the enrollment capacity of the Central Department of Chemistry and other Campuses.

Course Structure:

The entire Master of Science (M. Sc.) in Chemistry is divided into four semesters (Two semesters/year) in two academic years. A two year (four semesters) Master's Degree under the semester system is equivalent to total of 70 credit hours and according to which a student must complete 70 credit hours courses to earn Master's Degree in Chemistry. There will be 15 working weeks in a semester. A regular student is required to take 15-21 credit hours per regular semester. The program will offer mandatory theory courses, advance theory courses, elective courses, practical courses and optional thesis work in chemistry. Throughout the semester, the program will follow a theory class (lecture) of 1 hour per week per credit hour. Six hours per week are allotted for the laboratory course carrying 2 credit hours, 15 hours per week are allotted for laboratory course carrying 5 credit hours and 18 hours per week are allotted for the dissertation and laboratory courses carrying 6 credit hours. There will be separate course number for each individual course.

The first two semesters offer core courses in inorganic/physical/organic chemistry each of which is equivalent to four credit hours (each group carries one credit hour), practical courses equivalent to 6 credit hours, 2 credit hours of research methodology in chemistry course and 1 credit hour term paper. The third semester offers the opportunity of choosing/specializing in one discipline out of three inorganic/physical/organic chemistry with an elective course. The theory and practical courses except an elective paper are of 4 credit hours and 5 credit hours, respectively. An elective paper is of 3 credit hours. A seminar of 1 credit hour will be held in the third semester and work load for the seminar will be as per the practical course.

In the fourth semester, there will be two advance courses of each 4 credit hours in each discipline and practical course or thesis of 6 credit hours.

Structure of M. Sc. Chemistry Syllabus (Semester System)-2017 (2073)

Semester	Course Title (Course Code)			Credit hours	Total
First	Inorganic Chemistry (CHE-501)			4	18
	Inorganic Chemistry Practical (CHE-502)			2	
	Physical Chemistry (CHE-503)			4	
	Physical Chemistry Practical (CHE-504)			2	
	Organic Chemistry (CHE-505)			4	
	Organic Chemistry Practical (CHE-506)			2	
Second	Inorganic Chemistry (CHE-551)			4	21
	Inorganic Chemistry Practical (CHE-552)			2	
	Physical Chemistry (CHE-553)			4	
	Physical Chemistry Practical (CHE-554)			2	
	Organic Chemistry (CHE-555)			4	
	Organic Chemistry Practical (Che-556)			2	
	Research Methodology in Chemistry (CHE-557a)			2	
	Term Paper in Chemistry (CHE-557b)			1	
Third	Inorganic Chemistry	Physical Chemistry	Organic Chemistry		17
	Inorganic Reaction Mechanism, Techniques and Inorganic Polymers (CHE-601)	Quantum Chemistry and Statistical Mechanics (CHE-604)	Organic Synthesis (CHE-607)	4	
	Selected Topics in Inorganic Chemistry (CHE-602)	Advanced Solid State Chemistry (CHE-605)	Organic Reaction Mechanism (CHE-608)	4	
	Inorganic Chemistry Practical (CHE-603a)	Physical Chemistry Practical (CHE-606a)	Organic Chemistry Practical (CHE-609a)	5	
	Inorganic Chemistry Seminar (CHE-603b)	Physical Chemistry Seminar	Organic Chemistry Seminar	1	

		(CHE-606b)	(CHE-609b)		
	Elective papers (CHE-610-to- CHE-615)	Elective papers (CHE-610-to- CHE-615)	Elective papers (CHE-610-to- CHE-615)	3	

Semester	Course Title (Course Code)			Credit hours	
Fourth	Inorganic Chemistry	Physical Chemistry	Organic Chemistry		14
	Bio-Inorganic Chemistry (CHE-651)	Advanced Electrochemistry and Corrosion Science (CHE-655)	Organic Stereochemistry (CHE-659)	4	
	Structure and Bonding in Complexes (CHE-652)	Molecular Spectroscopy (CHE-656)	Organic Spectroscopy (CHE-660)	4	
	Inorganic Chemistry Practical (CHE-653) OR Inorganic Chemistry Dissertation (CHE-654)	Physical Chemistry Practical (CHE-657) OR Physical Chemistry Dissertation (CHE-658)	Organic Chemistry Practical (CHE-661) OR Organic Chemistry Dissertation (CHE-662)	6 OR 6	
Total Credit Hours					70

Visit to industries or educational institutes will be arranged as deemed necessary, as a part of extracurricular activities.

Hours of Instruction:

- a. Working days: 90 days per semester.
- b. Class hour:

Theory: One theory paper of 4 credit hours will have 4 hours lecture per week.

Practical: One practical paper of 2 credit hours will have 6 hours of practical per week and that of 6 credit hours will have maximum up to 18 hours of practical per week and so on.

Attendance: 80 percent attendance in the class is mandatory.

Examination:

There will be two types of examinations in each semester one of which will be held by the IOST, Dean Office that carries the weightage of 60 % and 40 % internal evaluation will be held by the Department/Campuses. The internal evaluation will be made by taking two written examinations mid term and final term and student attendance.

The detailed course structure is as follows:

First Semester:

Subjects	Course Code	Credit Hours	Full Marks	Pass Marks
Inorganic Chemistry	CHE-501	4	100	50
Inorganic Chemistry Practical	CHE-502	2	50	25
Physical Chemistry	CHE-503	4	100	50
Physical Chemistry Practical	CHE-504	2	50	25
Organic Chemistry	CHE-505	4	100	50
Organic Chemistry Practical	CHE-506	2	50	25

Second Semester:

Subjects	Course Code	Credit Hours	Full Marks	Pass Marks
Inorganic Chemistry	CHE-551	4	100	50
Inorganic Chemistry Practical	CHE-552	2	50	25
Physical Chemistry	CHE-553	4	100	50
Physical Chemistry Practical	CHE-554	2	50	25
Organic Chemistry	CHE-555	4	100	50
Organic Chemistry Practical	CHE-556	2	50	25
Research Methodology in Chemistry	CHE-557a	2	50	25
Term Paper in Chemistry	CHE-557b	1	25	12.5

A work load equivalent to 2 periods will be allotted to the supervisor who supervises the term paper of each student.

On completion of M. Sc. second semester, the students will have the option of specializing either in inorganic or physical or organic chemistry in M. Sc. third and fourth semesters.

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.

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	CHE-653	6	150	75
OR	OR	OR	OR	OR
Inorganic Chemistry Dissertation	CHE-654	6	150	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	CHE-657	6	150	75
OR	OR	OR	OR	OR
Physical Chemistry Dissertation	CHE-658	6	150	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	CHE-661	6	150	75
OR	OR	OR	OR	OR
Organic Chemistry Dissertation	CHE-662	6	150	75

Inorganic Chemistry

Course Title: Inorganic Chemistry (Theory)

Credit: Four (4) hrs.

Course No.: CHE-501

Full Marks: 100

Semester: First (1st)

Pass Marks: 50

Course Objectives:

- ❖ To provide a broad knowledge of the advanced inorganic chemistry and the principles of qualitative and quantitative analysis.

Course Contents:

Group A

Atomic Structure: Review lecture, Schrödinger wave equation, interpretation of the wave function, normalized and orthogonal wave functions, the principle of superposition, the particle in a one dimensional box, the particle in a three dimensional box, degeneracy, the hydrogen atom, transformation of coordinates, separation of variables, the Φ equation, the θ equation, spherical harmonics, the radial equation, quantum states, electron spin, energy states of the hydrogen atom, the self-consistent-field method, wave functions of the hydrogen atom, radial distribution curves, angular dependence of the wave function, atomic spectra and term symbols.

Group B

Covalent Bond: The variation method, ground state energy of hydrogen atom, the Secular equations, non crossing rule.

Hybridization: sp^3 hybridization, hybridization with d orbitals d^2sp^3 and dsp^2 hybridization, trigonal and diagonal hybrids, non equivalent hybrids, relative strength and angular distribution of hybrid orbitals, contours plots of hybrid orbitals, construction of hybrid orbitals, the effect of unshared pair on hybridization.

Group C

Molecular Orbital Theory: Molecular orbitals and its types, LCAO approximation, significance of resonance integral, hydrogen molecule ion (H_2^+), hydrogen molecule (H_2), other homonuclear diatomics, heteronuclear diatomics, experimental determination of molecular structure.

Valence Bond Theory: Valence bond method, hydrogen molecule (H_2), other homonuclear diatomics, heteronuclear diatomics, quantum mechanical structure and the meaning of resonance.

Group D

Analytical and Instrumental: A brief review on chemical analysis. Redox titration: use of potassium bromate, ceric salts, redox indicators, complexometric titration: metal ion indicators, adsorption titration: adsorption indicators, uses of common organic reagent in chemical analysis (dmg, oxine, cupferron).

Instrumentation, working principles and applications of following spectroscopic techniques: atomic absorption spectroscopy, atomic emission spectroscopy: flame photometry, atomic fluorescence spectroscopy, plasma emission spectroscopy (direct current plasma and inductively coupled plasma), molecular luminescence: fluorescence and phosphorescence, thermal analysis: thermo-gravimetric analysis (T.G.A), differential thermal analysis (D.T.A).

Reference Books for CHE-501:

1. F. A. Cottton and G. Wilkinson, *Advanced Inorganic Chemistry* (5th Edition) John Wiley and Sons Ins., 1988.
2. F. A. Cottton and G. Wilkinson and Paul L. Gauss, *Basic Inorganic Chemistry* (3rd Edition), John Wiley and Sons Incorporation, 1995.
3. J. E. Huheey, Ellen A. Keiter and Richard L. Keiter, *Inorganic Chemistry* (4th Edition), Harper Collins College Publishers, 1993.
4. J. Mendharm, R.C. Denny, J.D. Branes and M. Thomas, *Vogel's Textbook of Quantitative Chemical Analysis*, (6th Edition), 2008.
5. C. A Coulson, *Valence*, E.L.B.S., (2nd Edition), 1975.
6. M. C. Day and J. Selbin, *Theoretical Inorganic Chemistry*, East-west Press Pvt. Ltd., 1985.

7. G. L. Miessler and D. A. Tarr, *Inorganic Chemistry*, (5th Edition), 2014.
8. D. F. Shriver and P. W. Atkins, *Inorganic Chemistry*, (5th Edition) Oxford University Press.
9. D. A. Skoog, *Principle of Instrumental Analysis*, (3rd Edition), Saunders College Publishing, 1985.
10. H. H. Willard, L. L. Merritt, J. R. Dean and F. A. Settle, *Instrumental Methods of Analysis* (7th Edition), CBS Publishers and Distributions, India, 1986.
11. R. A. Day and A. L. Underwood, *Quantitative Analysis* (6th Edition), Prentice-Hall of India, 1993.
12. A. F. Wells, *Structural Inorganic Chemistry*, (4th Edition) Clarendon, Oxford, 1975.
13. P. J. Durrant and B. Durrant, *Introduction to Advanced Inorganic Chemistry*, Wiley (Interscience), (Latest Edition.), New York.
14. L. Pauling, *The Nature of the Chemical Bond* (Latest Edition), Cornell University Press.
15. R. McWeeny, *Coulson's Valence*, Oxford Press, 1979.
16. E. Cartmell and G.W. A. Fowles, *Valency and Molecular Structure* (4th Edition), Butterworth , 1997.
17. Bodie Douglas, Darl McDanniel and John Alexander, *Concepts and Models of Inorganic Chemistry*, (3rd Edition), John Wiley and Sons Inc., 1994.
18. G. H. Jeffery, J. Bassett, J. Mendharm and R. C. Denny, *Vogel's Textbook of Quantitative Chemical Analysis*, E.L.B.S., 1994.
19. F.A. Cotton, G. Wilkinson, C.A. Murillo and Manfred Bochmann , *Advanced Inorganic Chemistry*, (6th Edition), John Wiley and Sons, 1999.

Inorganic Chemistry

Course Title: Inorganic Chemistry Practical

Credit: Four (2) hrs.

Course No.: CHE-502

Full Marks: 50

Semester: First (1st)

Pass Marks: 25

Course Objective:

- ❖ To acquaint the students with quantitative and qualitative analytical methods.

Course contents:

Volumetric Analysis:

1. Determination of ferrous and ferric ions in a given mixture by potassium dichromate solution.
2. Determination of copper and iron in a given mixture by potassium dichromate solution.
3. Determination of percentage purity of pyrolusite by arsenious oxide.
4. Determination of copper as oxinate in the given copper sulphate solution by using potassium bromate.
5. Determination of percentage of "available chlorine" in bleaching powder by using potassium bromate.
6. Determination of zinc as oxinate in the given zinc sulphate solution by using potassium bromate.
7. Standardization of silver nitrate with the help of standard sodium chloride solution by Mohr's method.
8. Determination of amount of NaCl and KCl [and KCl and KBr] in a mixture by silver nitrate.
9. Determination of percentage purity of potassium bromide by using adsorption indicator.
10. Determination of amount of calcium, magnesium and manganese in a mixture by the use of EDTA.
11. Determination of hardness of water.

12. Determination of amount of copper and zinc in a mixture by EDTA.

13. Determination of total iron in a given sample of water.

14. Determination of ammonia in a given sample of water.

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

Reference Books for CHE-502:

1. M.R. Pokhrel, P.N. Yadav and S. Shrestha, *Advanced Practical Inorganic Chemistry for M.Sc.*, (2nd 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. Saunders Co. (Saunders Golden Series), Philadelphia, 1991.
5. K. N. Ghimire, M. R. Pokhrel & K. P. Bohara, *University Experimental Inorganic Chemistry*, Quest Publication, Kirtipur, Kathmandu, 2008.

Physical Chemistry

Course Title: Physical Chemistry (Theory)

Credit: Four (4) hrs.

Course No.: CHE-503

Full Mark: 100

Semester: First (1st)

Pass Mark: 50

Course Objectives:

- ❖ To introduce the basic concepts on advanced techniques for surface analysis of solids
- ❖ To provide knowledge on electro-analytical techniques, chemical kinetics & group theory

Course Contents:

Group A

Advanced Surface Characterization Techniques: Introduction of solid surfaces, *electron emission spectroscopic and imaging microscopic techniques*; *X-ray photoelectron spectroscopy (XPS)*: introduction, basic principle, instrumentation, XPS spectra, applications, advantages and limitations; basic principle, instrumentation, advantages and limitations of *Angle-resolved XPS (ARXPS)* and *Auger electron spectroscopy (AES)*; comparison between XPS and AES; *scanning electron microscopy (SEM)*: introduction, basic principle, types of emitted electron for SEM, instrumentation, applications, advantages and limitations; *scanning probe microscopy (SPM)*: introduction, general principle of SPM, principle of scanning tunneling microscopy (STM), principle of atomic force microscopy (AFM), instrumentation of STM and AFM, different modes of STM and AFM, applications, advantages and limitations of SPM; *transmission electron microscopy (TEM)*: introduction, basic principle, modes, instrumentation, application advantages and limitations.

Group B

Electro-analytical Methods: Definition and classification of electro-analytical methods; basic principles of voltammetry; principal, instrumentation, applications and limitations

of DC polarography, pulse voltammetry (normal pulse, differential pulse, square wave), cyclic voltammetry, stripping voltammetry, AC voltammetry, amperometry (one electrode and two electrode system), Karl Fisher titration, coulometry, electrogravimetry and ion-selective electrodes (glass and solid state).

Group C

Chemical Kinetics: *Methods of fast reaction kinetics:* flow, relaxation, flash photolysis; *Polymerization kinetics:* derivation of rate equation for molecular and free radical mechanisms, cationic, anionic and emulsion polymerizations, related numericals; *Enzyme catalyzed reaction kinetics:* Michaelis-Menten mechanism of enzyme action, derivation of rate equation, graphical representations; influence of pH and temperature in enzyme action & related numericals; *Oscillating reaction kinetics:* introduction, Lotka-Volterra mechanism of chemical oscillation; *Diffusion controlled reactions in solution:* introduction, kinetics of diffusion-controlled reactions, kinetic salt effect, electron transfer reaction, potential energy surfaces; attractive and repulsive surfaces; classical trajectories: brief explanation with curve; related numericals.

Group D

Group Theory for Chemistry: Concept of Group Theory, group multiplication tables, cyclic and abelian groups, subgroups, similarity transforms, classes, symmetry elements, symmetry operations as group elements, consequences of symmetry, systematic classification of molecules into point group, matrix representations of symmetry operations and groups, reducible and irreducible representations, greater orthogonality theorem, character tables, properties of character tables and reduction formula, bond vectors and mathematical functions as bases for representations, basic concept of applications of group theory in chemical bonding and normal mode of molecular vibration (IR and Raman).

Reference Books for CHE-503:

1. C. R. Brundle, C. K. Evans, Jr., S. Wilson and L. E. Fitzpatrick (eds), *Encyclopedia of Materials Characterization: Surfaces, Interfaces, Thin Films*, Butterworth-Heinemann, Reed Publishing (USA) Inc., 1992.
2. J. Bhattarai, *Frontiers of Surface Analysis*, (1st Edition), Balkhu, Kathmandu, Nepal.

- 2012.
3. C. D. Wagner, W. M. Riggs, L. E. Davis, J. F. Moulder and G. F. Mullenburge (eds), *Handbook of X-ray Photoelectron Spectroscopy*, Perkin-Elmer Co. Minnesota, USA, 1979.
 4. J. Bhattarai, *Introduction to Electron Spectroscopy for In-depth Surface Analysis*, (1st Edition), Balkhu, Kathmandu, Nepal, 2011.
 5. J. O'M. Bockris, A. K. N. Reddy and M. Gamboa-Aldeco, *Modern Electrochemistry, Fundamentals of Electrodeics*, (2nd Edition), Vol. 2A, Kluwer Academic/Plenum Publishers, New York, 2000.
 6. A. J. Bard and L. R. Faulkner, *Electrochemical Methods: Fundamentals and Applications*, (2nd Edition), John Wiley & Sons Inc., New York, 2001.
 7. *Vogel's Textbook of Quantitative Inorganic Analysis*, (4th Edition), ELBS/Longman Scientific & Technical, London, 1978 (or more recent edition).
 8. D. A. Skoog, D. M. West, F. J. Holler and S. R. Crouch, *Fundamentals of Analytical Chemistry*, (8th Edition), International Student edition, Books/Cole Cengage Learning, Belmont, USA, 2004.
 9. K. J. Laidler, *Chemical Kinetics*, Harper and Row, New York, 1988.
 10. G. K. Vemulapalli, *Physical Chemistry*, Prentice-Hall of India Pvt. Ltd., New Delhi, 1997.
 11. P. Atkins & J. de Paula, *Atkins' Physical Chemistry*, (10th Edition), Oxford University Press, New Delhi, 2014.
 12. D. A. McQuarrie and J. D. Simon, *Physical Chemistry: a Molecular Approach*, Viva Student Edition, Viva Books Pvt. Ltd., New Delhi, 2011.
 13. F. A. Cotton, *Chemical Applications of Group Theory*, (3rd Edition), John Wiley & Sons Inc., New York, 1990.
 14. A. Salahuddin Kunju and G. Krishnan, *Group Theory and its Applications in Chemistry*, PHI learning Pvt. Ltd., New Delhi, 2010.

Physical Chemistry

Course Title: Physical Chemistry Practical

Credit: Two (2) hrs.

Course No.: CHE-504

Full Mark: 50

Semester: First (1st)

Pass Mark: 25

Course Objective:

- ❖ To make students capable of conducting physical chemistry experiments and analysis the data.

Course Contents:

Electrochemistry

1. Analyze the mixture of H_2SO_4 , CH_3COOH and CuSO_4 with sodium hydroxide solution by conductometric method.
2. Determination of solubility product of sparingly soluble salt (BaSO_4) by conductometric method.
3. Potentiometric titration of a mixture of KCl and KI solutions and determine the concentration of KCl and KI solutions.
4. Preparation of standard buffer solution of CH_3COOH and CH_3COONa (pH 3.6, 4.0, 4.4, 4.8 & 5.2) and measure the solution pH using glass electrode and hence find out Nernstian slope.
5. Preparation of different buffer solutions using NH_4Cl and NH_4OH and measure the pH of solution by pH-meter using glass electrode and hence verify Henderson equation.

Chemical Kinetics

6. Energy of activation of acid catalyzed hydrolysis of methyl acetate.
7. Find the activation energy and the study the influence of ionic strength on the rate constant of reaction between $\text{K}_2\text{S}_4\text{O}_8$ and KI solutions.
8. Kinetics of the oxidation of iodide ions by H_2O_2 as an iodine clock reaction.

Miscellaneous

9. Calibration of common volumetric glass wares; pipette, burette and measuring cylinder.
10. Determine the enthalpy of neutralization of weak acid and strong base by using coffee cup calorimeter.
11. Determination of cross sectional area of $-\text{COOH}$ group by measuring the variation of surface tension with concentration of butyric acid.
12. Plot current-voltage curves for given solutions of CuSO_4 and H_2SO_4 using platinum electrodes
13. Titration of iodine solution with sodium thiosulphate solution by the dead stop end point method or polarization method.

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

Reference Books for CHE-504:

1. J. N. Gurtu and A. Gurtu, *Advanced Physical Chemistry Experiments*, (6th Edition), Pragati Prakashan, Meerut, India, 2014.
2. M. K. Sthapit and R. R. Pradhananga, *Experimental Physical Chemistry*, Taleju Prakashan, Kathmandu, 1998.
3. *Findlay's Practical Physical Chemistry*, (9th Edition), revised by B. P. Levitt, Longman Group Ltd., London, 1973.
4. D. B. Khadka, *Practical Physical Chemistry*, Sunlight Publication (Student's Book), Kathmandu, 2009.

Organic Chemistry

Course Title: Organic Chemistry (Theory)

Credit: Four (4) hrs.

Course No.: CHE-505

Full marks: 100

Semester: First (1st)

Pass marks: 50

Course Objectives:

- ❖ To provide the students basic knowledge about reaction mechanism.
- ❖ To familiarize important organic reagents used in synthesis.
- ❖ To acquaint the students with modern synthetic reactions.
- ❖ To provide the students basic knowledge of photochemistry.

Course Objectives:

Group A

Acids and Bases: Bronsted theory, the origin of acidity in organic compounds (factors influencing the acidity of an organic compounds), the mechanism of proton transfer reactions, acids and base solvents, measurement of solvent acidity (no mathematical derivation), acid and base catalysis (general and specific), Bronsted and Marcus equation, Lewis acids and bases, hard and soft acids and bases, the effects of structure on the strengths of acids and bases, effect of medium on acid and base strength.

Effects of Structure on Reactivity: Resonance and field effects, steric effects, quantitative treatments of the effect of structure on reactivity (The Hammett equation), substituent constant σ_x , reaction constant ρ , physical significance of σ_x , physical significance of ρ , uses of Hammett plots.

Group B

Aliphatic Nucleophilic Substitution: Review lecture (S_N1 and S_N2 reaction and mechanism with suitable examples, the neighboring-group mechanism, the neighboring-group participation by sigma and pi bonds, non-classical carbocations), ion-pairs in the S_N1 mechanism, mixed S_N1 and S_N2 reactions, SET mechanism, nucleophilic

substitution at allylic carbon, nucleophilic substitution at vinylic carbon, nucleophilic substitution at a trigonal carbon, S_{Ni} reaction and mechanism.

Aromatic Nucleophilic Substitution: Introduction, S_{NAr} mechanism, the S_{N1} mechanism, S_{RN1} mechanism, the benzyne mechanism.

Aromatic Electrophilic Substitution: Arenium ion mechanism, evidences for the arenium ion mechanism, the S_{E1} mechanism, orientation and reactivity in mono substituted benzene ring, ortho/para ratio, Ipso attack.

Aliphatic Electrophilic Substitution: Mechanisms, bimolecular mechanism S_{E2} and S_{Ei} mechanism, S_{E1} mechanism with suitable examples, electrophilic substitution accompanied by double bond shift.

Free Radical Substitution: Mechanisms, Free radical mechanism in general, free radical mechanism, mechanisms at an aromatic substrate, neighboring group assistance in free Radical Reactions, allylic halogenations.

Group C

Elimination Reaction: Review lecture, The $E1$ mechanism, $E2$ mechanism, $E1cB$ mechanism, the $E2c$ mechanism, the $E1$ - $E2$ - $E1$ CB spectrum, steric orientation of the double bond, reactivity– effect of substrate, structure, effect of attacking base, effect of leaving group, effect of the medium, mechanism and orientation in pyrolytic elimination, orientation of double bonds.

Synthetic Reactions and Reagents: Carbon-carbon bond forming reactions of organometallic reagents.

Carbon-carbon double bond forming reactions: Shapiro reaction, Bamford Steven reaction, Julia olefination reaction, Petersion chain olefination reaction.

Carbon-heteromultiple bond forming reactions: Passerini and Ugi reaction, Mannich reaction

Ring forming reactions: Pauson-Khand reaction, Demjenov cyclization.

Other synthetic reactions: Eschemoser-Tanabe ring cleavage reaction, Mitsunobu reaction, Stork enamine reaction, Michael reaction.

Group D

Photochemistry: Introduction, thermal and photochemical energy, activation energy, photochemical excitation, electronic transition, Jablonski diagrams, intersystem crossing,

photolytic cleavage, laws of photochemistry, quantum yield, photochemistry of carbonyl compounds, Norrish Type I and II-reactions, Paterno Buchii reaction, olefine photochemistry, photo dimerization, photoreduction of carbonyl compounds, photochemical oxidation, photo-rearrangement, photochemistry of α -, β -unsaturated ketones, photochemistry of aromatic compounds, introduction to electrocyclic reaction and cycloaddition.

Reference Books for CHE-505:

1. J. March, *Advanced Organic Chemistry*, (4th Edition), John Wiley and Sons, 1992.
2. Michael B. Smith, *March's Advanced Organic Chemistry*, (7th Edition), John Wiley and Sons, Inc., 2013.
3. Charles DePuy and Orville L. Chapman, *Molecular Reaction and Photochemistry*, Prentice-Hall, 1972.
4. I. L. Finar, *Organic Chemistry*, Vols. 1 and 2, ELBS, 1975.
5. Seyhan Ege, *Organic Chemistry Structure and Reactivity*, (3rd Edition), A.I.T.B.S. Publishers & Distributors, 1999.
6. Peter Sykes, *A Guide Book to Mechanism in Organic Chemistry*, (6th Edition), Pearson.
7. Education, Singapore, 1986.
8. R. Norman and J. M. Coxon, *Principles of Organic Synthesis*, CRC/CBS Publishers & Distributors, 1993.
9. I. Kumar, *Organometallic Compounds*, (5th Edition), Pragati Prakashan, Meerut, India, 2015.
10. J. Clayden, N. Greeves, and S. Warren, *Organic Chemistry*, (2nd Edition), Oxford University Press, India, 2014.

Organic Chemistry

Course Title: Organic Chemistry Practical

Credit: Two (2) hrs.

Course No.: CHE-506

Full Marks: 50

Semester: First (1st)

Pass Marks: 25

Course Objective:

- ❖ To train the students in handling different equipments and train them further in identification, isolation and preparation of different compounds.

Course Contents:

1. Purification and drying of solvents and chemicals.
2. Experiments on chromatography.
3. An experiment on mixed melting point.
4. Identification of organic compounds containing mono and bifunctional groups such as aldehyde, ketone, carboxylic acid, ester, carbohydrate, phenol, hydrocarbon, amino group, nitro group, amide, ammonium salt etc and preparation of two derivatives for each.
5. Experiments on photochemistry.

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

Reference Books for CHE-506:

1. N. K. Vishnoi, *Advanced Practical Organic Chemistry* (3rd Edition), Vikas Publishing House 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.

Inorganic Chemistry

Course Title: Inorganic Chemistry (Theory)

Credit: Four (4) hrs.

Course No.: CHE-551

Full Marks: 100

Semester: Second (2nd)

Pass Marks: 50

Course Objective:

- ❖ To provide a broad knowledge of the advanced Inorganic Chemistry.

Course Contents:

Group A

Co-ordination Compounds: Crystal field theory, splitting of orbitals in different geometries using group theory, crystal field stabilization energy, explanation of spectrochemical series, limitations and uses of CFT, Evidences for covalent bonding in complex and nephelauxetic series, thermodynamic effect of CFSE, enthalpies of hydration and free energy, lattice energies, Jahn Teller effect, dynamic Jahn Teller behavior, explanation of magnetic properties, colour of transition metal complexes, characterization of coordination compounds, different spectroscopic and analytical techniques.

Group B

Acid Base Chemistry: Review of acid base concept, generalized acid-base concept, measures of acid base strength, Lewis interaction in non polar solvents, systematic of Lewis acid-base interaction, bond energies, steric effects, proton sponges, solvation effect, and acid-base anomalies, acid-base strength and hardness and softness, electronegativity and hardness and softness, MC-Daniel diagram, super acids and super bases.

Chromatography: Size exclusion chromatography, ion exclusion chromatography, ion-retardation chromatography, inorganic molecular sieves.

Isoelectronic and Isolobal Relationship: Isoelectronic species, criteria for isolobality, organic and organometallic isolobal fragments, extension of isolobal analogy, importance of the concept of isolobality.

Supra Molecular Chemistry: Molecular recognition, transformation and translocation, supra molecules, supra molecular assemblies, factors affecting molecular recognition, crown ethers, cryptands, mesoporous materials, inorganic-organic nanocomposites catalysis.

Group C

Buckminster Fullerene: Introduction, preparation, structure, compounds formed by fullerene, higher fullerenes.

Nanochemistry: Fundamentals of nanochemistry, building blocks, concepts of quantum dots, tools of nanotechnology (AFM, SEM, TEM, STM), applications and toxicity of nanomaterials.

Carbon Nanotubes: Introduction, types of carbon nanotubes, different synthesis techniques of carbon nanotubes, applications.

Radio-activity and Nuclear Reaction: Characteristics of nuclear reactions and their similarity with chemical reactions, nuclear reactors, types of nuclear reactors, classification of reactors, fission probability, process yield and applications and fall out, units and measurement of radioactivity and radiation, activation analysis, ^{14}C dating, tracer technique, radiochemical analysis.

Group D

Cement: Manufacture, composition of cement, Portland cement, types of cement, concrete, additive, hydration process.

Ceramics: Types of ceramics, glass, structural characteristics, glass transition temperature, composition, production and application, optical fibres, electrochromism, photochromism.

Zeolites: Molecular sieves, zeolite aluminosilicate, structure of zeolites, synthesis of zeolites, applications of zeolites, composition and properties of zeolites, zeolites as shape selective heterogenous catalyst.

Intercalation Chemistry: Types of intercalation compound, graphite intercalation compounds, layered silicate structures, applications.

One Dimensional Conductors: Polythiazyls (polymeric sulphur nitride), structural characteristics, stacked columnar complexes.

Isopolyanions and Heteropolyanions: Structural characteristic, variation of composition with pH value.

Reference Books for CHE-551:

1. F. A. Cotton and G. Wilkinson, *Advanced Inorganic Chemistry* (5th Edition) John Wiley and Sons Ins., 1988.
2. F. A. Cotton and G. Wilkinson and Paul L. Gaus, *Basic Inorganic Chemistry* (3rd Edition), John Wiley and Sons Incorporation, 1995.
3. J. E. Huheey, Ellen A. Keiter and Richard L. Keiter, *Inorganic Chemistry* (4th Edition), Harper Collins College Publishers, 1993.
4. Bodie Douglas, Darl McDaniell and John Alexander, *Concepts and Models of Inorganic Chemistry* (3rd Edition), John Wiley and Sons Incorporation, 1994.
5. G. L. Miessler and D. A. Tarr, *Inorganic Chemistry*, (5th Edition).
6. D.F. Shriver and P.W. Atkins, *Inorganic Chemistry*, (5th Edition), Oxford University Press.
7. A.F. Wells, *Structural Inorganic Chemistry*, (4th Edition) Clarendon, Oxford, 1975.
8. P. J. Durrant and B. Durrant, *Introduction to Advanced Inorganic Chemistry*, (Latest Edition), Wiley (Interscience), New York.
9. L. Pauling, *The Nature of the Chemical Bond* (Latest Edition), Cornell University Press.
10. G.H. Jeffery, J. Bassett, J. Mendharm and R. C. Denny, *Vogel's Textbook of Quantitative Chemical Analysis*, E.L.B.S., 1994.
11. R.A. Day and A.L. Underwood, *Quantitative Analysis*, (6th Edition), Prentice-Hall of India, 1993.
12. Satya Prakash, G.D. Tuli, S.K. Basu and R.D. Madan, *Advanced Inorganic Chemistry* (Vol. II), (Reprinted Edition), S. Chand Publishing, 2013.

Inorganic Chemistry

Course Title: Inorganic Chemistry Practical

Credit: Two (2) hrs.

Course No.: CHE-552

Full Marks: 50

Semester: Second (2nd)

Pass Marks: 25

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:

Gravimetric Analysis:

1. Estimation of copper as thiocyanate and zinc as pyrophosphate in a mixture of the two.
2. Estimation of Ca as oxide and Mg as pyrophosphate in a mixture of the two.

Salt Analysis:

Qualitative analysis of inorganic salt mixture containing 8 radicals excluding rare earth metals by semimicro method.

Preparations:

1. Preparation and characterization of hexaamminenickel(II) chloride, $[\text{Ni}(\text{NH}_3)_6]\text{Cl}_2$.
2. Preparation and characterization of potassium trioxalato chromate(III)
3. Preparation and characterization of cuprous thiourea complex.
4. Preparation of cuprous oxide and characterization.
5. Preparation and characterization of cuprous mercuric iodide, $\text{Cu}_2[\text{HgI}_4]$.
6. Preparation of about 6 to 8 complexes.

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

Reference Books for CHE-552:

1. M.R. Pokhrel, P.N. Yadav and S. Shrestha, *Advanced Practical Inorganic Chemistry for M.Sc.*, (2nd 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. Saunders Co. (Saunders Golden Series), Philadelphia, 1991.
5. K. N. Ghimire, M. R. Pokhrel & K. P. Bohara, *University Experimental Inorganic Chemistry*, Quest Publication, Kirtipur, Kathmandu, 2008.

Physical Chemistry

Course Title: Physical Chemistry (Theory)

Credit: Four (4) hrs.

Course No.: CHE-553

Full Mark: 100

Semester: Second (2nd)

Pass Mark: 50

Course Objectives:

- ❖ To provide knowledge on solid state chemistry, surface and colloidal chemistry, and thermodynamics
- ❖ To introduce about the structure of the electrified interfaces

Course Contents:

Group A

Solid State Chemistry: Chemical bonding in solids, lattice energies of ionic solids, structure of solids, determination of crystal structures, factors affecting crystal structure; classical free electron theory of metals, electrical conductivity, Ohm's law, Wiedemann-Franz ratio, heat capacity, conduction electrons, drawbacks of classical free electron theory; solid surfaces: surface forces, surface structure & surface composition.

Group B

Electrified Interfaces: Electrification of an interface; potential difference across electrified interfaces; accumulation and depletion of substances at an interface (concept of surface excess, determination of surface excess); thermodynamics of electrified interfaces (electro-capillary curve, Lippmann equation); quantitative treatment of electric double layer models (Helmholtz-Perrin, Gouy-Chapman, Stern, specific adsorption and complete-capacity models); structure of semiconductor-electrolyte interface: some *in situ* and *ex situ* techniques for studying electrified interface.

Group C

Chemistry of Surfaces & Colloids: *Adsorption:* Practical adsorbent materials; activated carbon and carbon molecular sieves; forces and energies of adsorption; calculation of heat of adsorption; adsorption at low coverage-Henry's law

Review lecture of Langmuir, Freundlich and BET adsorption isotherms; derivation of isotherms equation from Gibbs equation; adsorption mixtures; extended Langmuir model; Langmuir-Freundlich equations; Dubinin Polanyi theory; ideal adsorption solution theory; other model isotherms and their comparison.

Colloids: Importance of colloids and colloidal phenomena; mechanism of colloidal formation; roots of colloidal behavior; ground rules for colloidal stability; sources of colloidal stability; steric stabilization; coagulation kinetics; association colloids (micelles, vesicles and membranes); correlation between surfactant structure, environment and micellization.

Group D

Thermodynamics: Thermodynamic properties of solution: partial molar quantities; Gibbs-Duhem equation; chemical potential; chemical potential of pure substance; chemical potential of real gas and fugacity and its determination; chemical potential in ideal gas mixture; thermodynamics functions of mixing; properties of liquid solutions; colligative properties.

Non-equilibrium thermodynamics: limitations of classical thermodynamics, steady state or stationary state, principle of non-equilibrium thermodynamics; Onsager's reciprocity relations; entropy: production its rate in chemical and electro-chemical reaction; thermo-osmosis; electro-kinetic phenomenon.

Reference Books for CHE-553:

1. S. O. Pillai, *Solid State Chemistry*, Wiley Eastern Ltd., New Delhi, 1994.
2. P. Atkins and J. de Paula, *Atkins' Physical Chemistry* (10th Edition), Indian edition, Oxford University Press, 2014.
3. H. V. Keer, *Principles of the Solid State*, New Age Intl. Ltd., New Delhi, 2002.
4. J. Bhattarai and D. B. Khadka, *Surface Characterization and Solid State Chemistry*, (1st Edition), Sunlight Publication, Kirtipur, Kathmandu, 2010.
5. D. K. Chakrabarty, *Solid State Chemistry*, New Age Intl. Ltd., New Delhi, 1996.

6. J. O'M. Bockris, A. K. N. Reddy and M. Gamboa-Aldeco, *Modern Electrochemistry, Fundamentals of Electrodics*, (2nd Edition), **Vol. 2A**, Kluwer Academic/Plenum Publishers, New York, 2000.
7. A. J. Bard and L. R. Faulkner, *Electrochemical Methods: Fundamentals and Applications*, (2nd Edition), John Wiley & Sons Inc., New York, 2001.
8. R. P. Rastogi and R. R. Mishra, *An Introduction to Chemical Thermodynamics*, (6th Edition), Vikash Publ. House Pvt. Ltd., India, 1st reprint 2013.
9. G. K. Vemulapalli, *Physical Chemistry*, Prentice Hall of India, New Delhi (1997).
10. I. M. Klotz, *Chemical Thermodynamics*, Menlo Park, CA, 1986.
11. H. K. Moudgil, *Textbook of Physical Chemistry*, PHI Learning Pvt. Ltd., New Delhi, 2010.
12. S. Glasstone, *Theoretical Chemistry*, (1st Edition), D. Van Nostrand Company, Inc., New York, 1944.
13. Douglass M. Ruthven, *Principles of Adsorption and Adsorption Processes*, John Wiley & Sons, New York, 1984.
14. Drew Myers, *Surfaces, Interfaces and Colloids: Principles and Applications*, (2nd Edition), John Wiley & Sons, New York, 1999.

Physical Chemistry

Course Title: Physical Chemistry Practical

Credit: Two (2) hrs.

Course No.: CHE-554

Full Mark: 50

Semester: Second (2nd)

Pass Mark: 25

Course Objective:

- ❖ To make students capable of conducting physical chemistry experiments and analysis the data independently.

Course Contents:

Electrochemistry

1. Analyze the mixture of HCl, NH₄Cl and NaCl by conductometric titration.
2. Determine the equivalent conductivity of strong electrolytes at different dilutions and verify the Debye-Huckel-Onsager equation.
3. Potentiometric determination of solubility and solubility product of a sparingly soluble salt (AgCl) in water.
4. Potentiometric titration of phosphoric acid with sodium hydroxide using pH electrode (metal oxide or glass electrode) and find out the first and second dissociation constant of acid at room temperature.
5. Potentiometric titration of ferrous ammonium sulphate with potassium dichromate and determine the formal potential of Fe³⁺/Fe²⁺ system.
6. Potentiometric determination of equilibrium constant for the formation of complex ion [Ag(NH₃)₂]⁺.

Chemical Kinetics

7. Kinetic study of the saponification of ethyl acetate with sodium hydroxide by titration method.
8. Determination of total order of reaction between oxalic acid and chromic acid.

Surface Chemistry

9. Verification of Freundlich and Langmuir adsorption isotherms in adsorption process of oxalic acid onto activated charcoal and determine the specific surface area.
10. Study the variation of surface tension of solutions of n-propyl alcohol with concentration and determine the limiting cross-sectional area of alcohol molecule.

Spectrophotometry

11. Spectrophotometric determination of chromium (VI) by 1,5 diphenyl carbazide as a reagent for color development.
12. Determination of nitrite nitrogen in water using 1-naphthol and 4-aminophenylacetic acid as color developing reagent.

Miscellaneous

13. Determine of the equilibrium constant of $I_2 + KI \rightarrow KI_3$ reaction by distribution method.

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

Reference Books for CHE-554:

1. J. N. Gurtu and A. Gurtu, *Advanced Physical Chemistry Experiments*, (6th Edition), Pragati Prakashan, Meerut, India, 2014.
2. M. K. Sthapit and R. R. Pradhananga, *Experimental Physical Chemistry*, Taleju Prakashan, Kathmandu, 1998.
3. *Findlay's Practical Physical Chemistry*: (9th Edition), revised by B. P. Levitt, Longman Group Ltd., London, 1973.
4. D. B. Khadka, *Practical Physical Chemistry*, Sunlight Publication (Student's Book), Kathmandu, 2009.

Organic Chemistry

Course Title: Organic Chemistry (Theory)

Credit: Four (4) hrs.

Course No.: CHE-555

Full Marks: 100

Semester: Second (2nd)

Pass marks: 50

Course Objectives:

- ❖ To introduce macromolecular chemistry and supramolecules.
- ❖ To acquaint with different aspects of stereochemistry.
- ❖ To acquaint with heterocyclic, carbohydrate and carbocyclic chemistry.
- ❖ To provide fundamental knowledge about natural product chemistry.
- ❖ To provide basic knowledge about chromatographic and spectroscopic techniques.

Course Contents:

Group A

Macromolecular Chemistry: Introduction to macromolecules, type of polymerization, mechanism of chain growth polymerization, step growth polymerization, co-ordination polymerization, macromolecule of industrial importance (functional polymers, biomedical polymers (contact lens, dental polymers, artificial heart, kidney, skin and blood cells, special properties of large molecules (in terms of difference in behavior on heating, solubility pattern of low molecular weight compound and a polymer, reactions of polymer, stereoisomerism).

Supramolecular Chemistry: Introduction to supramolecular chemistry, concepts of supramolecular chemistry, examples of supramolecular compounds, uses, synthesis of Crown ethers and their uses, inclusion compounds.

Alicyclic Compounds: Synthesis of small rings (3-4 membered ring), medium sized rings (5-7) and large rings (above 8 members), structure elucidation and synthesis of muscone and civetone.

Group B

Stereochemistry:

Structure and symmetry: Symmetry introduction, symmetry elements, symmetry operators, symmetry points groups, point groups containing chiral molecules, point groups containing only achiral molecules, point groups corresponding to the platonic solids T_d , O_h , I_h .

Racemization and Methods of Resolution:

Racemization process: Thermal racemization, by anion formation, by cation formation, racemization via stable inactive intermediates, by chemical transformation, epimerization, mutarotation, and asymmetric transformation, acid catalyzed and base catalyzed processes, racemization of amino acids.

Racemates: Properties of racemates (m.p., solubility, vapour pressure), IR-spectra, NMR, chromatograph apical activity, Interaction with other chiral substances, biological properties, determination of enantiomer and diastereomer composition (isotope dilution method, kinetic method, NMR Methods based on diastereotopicity, NMR in chiral solvents).

Resolution: Chemical separation of enantiomers via diastereomers (tartaric acid resolution, resolution of α,β -unsaturated ketones, optical activation of menthone), separation via complexes and inclusion compounds, asymmetric transformations of diastereomers, general methods for the separation of diastereomers, kinetic resolution, enzymatic resolution, Cram's and Prelog's rule.

Group C

Heterocyclic Compounds: Introduction to heterocyclic compounds, reactions, synthesis and uses of oxirane, aziridine, azetidine, imidazole, thiazole, isoquinoline, indoles.

Carbohydrates: Disaccharides (determination the structure of maltose and sucrose), Introduction to oligosaccharides and polysaccharides.

Natural Product Chemistry: Introduction, scope of natural products chemistry, sources of natural products, extraction procedure, phytochemical screening.

Group D

Separation Techniques: Types of chromatography, theory of chromatography, instrumentation and applications of TLC, column chromatography, gas chromatography, HPLC, GC-MS, LC-MS.

Spectroscopic Techniques: Theory and application of IR, UV, Mass, ^1H - and ^{13}C -NMR.

Spectroscopic Analysis: Use of spectroscopic techniques in structure elucidation of simple organic compounds.

Reference Books for CHE-555:

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 Company, T M H edition 1975.
3. R. M. Silverstein, G. C. Bassler and T. C. Morrill; *Spectroscopic Identification of Organic Compounds*, John Wiley and Sons Inc, 1991.
4. J. Dyer, *Applications of Absorption Spectroscopy of Organic Compounds*, Prentice Hall, 1989.
5. D. Williams and I. Fleming, *Spectroscopic Methods in Organic Chemistry*, (6th Edition), McGraw Hill, 2007.
6. E. Heftmann, *Chromatography*, (2nd Edition), Reinhold, 1967.
7. I. L. Finar, *Organic Chemistry* Vol. 1 and Vol. 2, ELBS Longman, 1975.
8. E. A. Davidson, *Carbohydrate Chemistry*, Holt, Reinhard and Winston, 1967.
9. J. Singh and R. C. Dubey, *Organic Polymer Chemistry*, (2nd Revised Edition), Pragati Prakashan, 2009.
10. J. M. Lehn, *Supramolecular Chemistry*, VCH, Weinheim, 1995.
11. 11.V. R. Gowariker, N. V. Viswanathan and J. Sreedhar, *Polymer Science*, New Age International, first edition, 1986.
12. J. Mendham, R.C. Denney, J. D. Barnes, M.J.K. Thomas, *Vogel's Quantitative Chemical Analysis* (6th Edition), Prentice Hall, 2000.
13. S. M. Khopkar, *Basic Concepts of Analytical Chemistry*, New Age International, 1998.
14. K. R. Palak, *Stereochemistry*, Pairavi Prakashan, Kathmandu, Nepal, 2017.
15. Y. R. Sharma, *Elementary Organic Spectroscopy*, S. Chand and Company, New Delhi, 2013.

Organic Chemistry

Course Title: Organic Chemistry Practical

Credit: Two (2) hrs.

Course No.: CHE-556

Full marks: 50

Semester: Second (2nd)

Pass marks: 25

Course Objective:

- ❖ To train the students in handling different equipment's and train them synthesis of different compounds and isolation of natural products.

Course Contents:

1. Synthesis of different compounds involving not more than two steps.
2. An experiment based on the use of soxhelt extraction.
3. An experiment on solvent-solvent extraction.
4. Phytochemical screening for alkaloids, terpenes and flavonoids.
5. Isolation and purification of caffeine.
6. Isolation of an essential oil.
7. An experiment on ion-exchange chromatography.
8. An experiment on gas-liquid chromatography.
9. An experiment on HPLC.

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

References Books for CHE-556:

1. N. K. Vishnoi, *Advanced Practical Organic Chemistry* (3rd Edition), Vikas Publishing House 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.

Research Methodology in Chemistry

Course Title: Research Methodology in Chemistry (Theory)	Credit: Two (2) hrs.
Course No.: CHE-557a	Full marks: 50
Semester: Second (2 nd)	Pass marks: 25

Course Objective:

- ❖ To impart the students the knowledge of research methodology in chemistry.

Course Contents:

Group A

Distinctive Concept: Definition of research, importance of research, motivation in research, research methodology and research methods, purpose of research, classification of research, types of research, research approaches, research process, research design, scientific method of research.

Comparative Concepts: Comparative idea of research methodology, social sciences and natural sciences, physical sciences and biological sciences, different branches of chemistry e.g. inorganic, organic, physical, analytical, fundamental and applied field research, library research and laboratory research, research methodology in different areas of chemistry.

Literature Survey: Chemical literature (Chemical Abstracts Beilstein and chemistry journals), primary and secondary sources of chemical information eg journals, reviews, monographs, text books, modern techniques in chemical literature search e.g. use of internet, INSDOC, computers, software programs, etc., identification of research problem and proposal writing.

Group B

Tools and Techniques used in Research: Solvents, purification of solvent, drying agents, reagents, reagent preparation, special lab techniques and experimental setting, grades of reagent, cost factors, hazards due to chemicals, apparatus and reaction procedure, vacuum line technique, handling of air sensitive compounds and hazardous chemicals, chromatographic techniques, spectroscopic techniques, chemical and physical techniques, high and low pressure techniques, techniques to study fast reaction, high and low temperature techniques, use of non-aqueous solvents.

Analysis of Research Finding: Analysis involved in data base research findings e.g., sampling, precision, accuracy, reproducibility, checking reproducibility of results, deviation, standard deviation, regression analysis, confidence limit, data analysis through computers, simple program development in chemical research, interpretation skill regarding spectroscopic data e.g. UV, IR, ¹HNMR, ¹³CNMR, Mass, GC-MS and X-ray-crystallography and different chromatograms.

Research Paper, Report and Thesis Writing: Format development, penmanship: variation in the format of report writing, drilling exercise in report writing and paper writing, citation of the references, bibliography.

References Books for CHE-557a:

1. S. P. Dhoubhadel, *Research Methodology in Chemistry*, Curriculum Development Centre, Tribhuvan University, Kirtipur, Kathmandu, 2002.
2. G. H. Jafferyetal, *Text book of Quantitative Chemical Analysis*; ELBS, Langman Group UK Ltd., 1989.
3. R. B. Bates and J. P. Schaefer, *Research Technique in Organic Chemistry*; Prentice Hall of India, 1971.
4. Paul Stapleton, *Writing Research paper; an Easy Guide for Non-native English Speaker*, ACIAR, Canberra, 1990.
5. R. J. Angelici, *Synthesis and Technique in Inorganic Chemistry*; W.B. Saunders Company (Saunders Golden Series), Philadelphia, 1977.
6. J. March, *Advanced organic Chemistry*, (4th Edition), John Wiley and Sons, 1992.

Term Paper

Course Title: Term Paper in Chemistry

Credit: One (1) hr.

Course No.: CHE-557b

Full marks: 25

Semester: Second (2nd)

Pass marks: 12.5

Course Objective:

- ❖ To make the students familiar with the original research papers published in peer reviewed chemistry journals.

Course Contents:

The students have to write and submit a term paper in the 2nd Semester on the topic provided by supervisor selecting at least five recent research papers published in peer reviewed chemistry journals. The format of the term paper and submission date will be provided by Central Department of Chemistry/Campuses.

Inorganic Chemistry

Course Title: Inorganic Reaction Mechanism,
Techniques and Inorganic Polymers (Theory)

Course No.: CHE-601

Semester: Third (3rd)

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 $[\text{Ru}(\text{bipy})_3]^{2+}$ 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*, (2nd Edition), Wiley Western Limited.

2. R.B. Jordan, *Reaction Mechanisms of Inorganic and Organo Metallic Systems*, (3rd 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*, (4th Edition), Addition-Wishley Publishing Company, 1993.
5. 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.
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*, (2nd 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. Langford 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, Oxford.
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. Zeldin, 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 Cliffs, 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.

Full Marks: 100

Course No.: CHE-602

Pass Marks: 50

Semester: Third (3rd)

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, chevreton 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, fluxional 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 (3rd)

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. Saunders Co. (Saunders Golden Series), Philadelphia, 1991.
3. M.R. Pokhrel, P.N. Yadav and S. Shrestha, *Advanced Practical Inorganic Chemistry for M.Sc.*, (2nd 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 (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.

Physical Chemistry

Course Title: Quantum Chemistry & Statistical Mechanics **Credit:** Four (4) hrs.
(Theory)

Course No.: CHE-604

Full Mark: 100

Semester: Third (3rd)

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 Intl. Ltd., New Delhi, 2002.
3. C. Kittel, *Introduction to Solid State Physics*, (8th 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*, (10th 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*, (1st Edition), Prentice-Hall Inc, New Jersey, 1973.
9. W. F. Smith and J. Hashemi, *Foundation of Materials Science and Engineering*, (4th Edition), McGraw-Hill, 2006.
10. V. Raghavan, *Materials Science and Engineering: a First Course*, (5th Edition), PHI Learning Pvt. Ltd., New Delhi, 2011.

Physical Chemistry

Course Title: Physical Chemistry Practical

Credit: Five (5) hrs.

Course No.: CHE-606a

Full Mark: 125

Semester: Third (3rd)

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 pK_a 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*, (6th 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.
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 (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.

Organic Chemistry

Course Title: Organic Synthesis (Theory)

Course No.: CHE-607

Semester: Third (3rd)

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:

- Reduction
- Oxidation
- Halogenation and alkylation
- 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 E₂ 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*, Pergamon 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, stereospecific and nonstereospecific 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 phosphoniummethyldes, phosphonatecarbanion and their reactions, generation of sulfonium and sulfoxoniummethyldes 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. nonconcerted cycloaddition, $\pi_2 + \pi_2$ cycloaddition, $\pi_2 + \pi_4$ cycloaddition, 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*, (4th 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 Winston, 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, *Structure 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 NaHCO₃, NaOH and HCl) as well as with water or ether or saturated solution of NaHSO₃. 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 enhancer (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*, Chapman and Hall, London. New York, 1990.
9. L. W. Aurand and A. E. Woods, *Food Chemistry*, The AVI publishing Co., Connecticut, 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 (3rd)

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, pentacyclitriterpenes, 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, oestrogen 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 B₁, B₁₂, 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*, Academic 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*, Chapman and Hall 1980.
12. H. Schmitterer, 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*, (6th Edition), Pragati Prakashan, Meerut, India, 2015.

Elective Paper

Course Title: Nuclear Chemistry (Theory)

Course No.: CHE-612

Semester: Third (3rd)

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, stellar 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. Arnikaar, *Essentials of Nuclear Chemistry*, (4th 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)

Credit: Three (3) hrs.

Course No.: CHE-613

Full Marks: 75

Semesters: Third (3rd)

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: ¹H-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., ¹⁹F, ³¹P, ¹⁵N and ¹¹B. Application in structural determination of simple organic and inorganic molecules; ¹³C-NMR: General introduction, peak assignments, chemical shift,

^{13}C - ^1H 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-stokes 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 (EI, CI, 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)

Credit: Three (3) hrs.

Course No.: CHE-614

Full Marks: 75

Semester: Third (3rd)

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 tandem 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 Stryer, *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 (3rd)

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.
2. J. Mendharm, R.C. Denny, J.D. Branes and M. Thomas, *Vogel's Textbook of Quantitative Chemical Analysis*, (6th Edition), 2008.
3. R. A. Day and A. L. Underwood, *Quantitative Analysis* (6th Edition), Prentice-Hall of India, 1993.
4. G. D. Christian, *Analytical Chemistry*, (5th Edition), John Wiley & Sons, New York, 1994.
5. D. A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, *Analytical Chemistry, An Introduction*, (7th Edition), Saunders College Publishing, Philadelphia, 2000.
6. S. M. Khopkar, *Basic Concepts of Analytical Chemistry*, (3rd Edition), New Age International Pvt. Ltd., New Delhi, India, 2008.
7. H. A. Laitinen and W. E. Harris, *Chemical Analysis*, (International Student Edition), McGraw Hill, Kogakusha, Ltd., 1975.

Inorganic Chemistry

Course Title: Bio-Inorganic Chemistry (Theory)

Credit: Four (4) hrs.

Course No.: CHE-651

Full Marks: 100

Semester: Fourth (4th)

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, transferrin, 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 B₁₂ and the B₁₂ 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 (4th)

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 ditechneium 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-ameridium elements, the super heavy elements.

Reference Books for CHE-652:

1. A.B.P. Lever, *Inorganic Electronic Spectroscopy*, (2nd 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. Langford 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*, (6th 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*, Pergamon 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

Credit: Six (6) hrs.

Course No.: Che-653

Full Marks: 150

Semester: Fourth (4th)

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 $\text{Co}(\text{NH}_3)_5\text{Cl}^{2+}$
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.*, (2nd 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. Saunders Co. (Sounders Golden Series), Philadelphia, 1991.

Inorganic Chemistry

Course Title: Inorganic Chemistry Dissertation

Credit: Six (6) hrs.

Course No.: CHE-654

Full Marks: 150

Semester: Fourth (4th)

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)

Credit: Four (4) hrs.

Full Mark: 100

Course No.: CHE-655

Pass Mark: 50

Semester: Fourth (4th)

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 CO₂, 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/H₂O systems; applications of potential-pH diagram for corrosion and its control with reference to Fe/H₂O 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 bands, 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. Herzberg, *Molecular Structure and Molecular Spectra: Vol. I 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 McGraw-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*, (10th Edition), Pragati Prakashan, Meerut, India, 2014.

Physical Chemistry

Course Title: Physical Chemistry Practical

Credit: Six (6) hrs.

Course No.: CHE-657

Full Mark: 150

Semester: Forth (4th)

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 $\text{C}_2\text{O}_4^{2-}$ 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*, (6th 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

Credit: Six (6) hrs.

Course No.: CHE-658

Full Mark: 150

Semester: Forth (4th)

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)

Credit: Four (4) hrs.

Course No.: CHE-659

Full Marks: 100

Semester: Fourth (4th)

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 polysubstituted cyclohexanes, 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, perhydrophenanthrene and perhydroanthracenes, bridged rings, Bredt's rule and bridge head alkenes, cryptands, crown ether, podands and spherands, paddlanes and propellanes, atenanes, rotanances, knots and Möbius 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), diastereoselective synthesis based on chiral substrates- (addition of nucleophile- Felkin transition states for addition of a nucleophile to cyclohexanone, electrophilic reactions of alkenes- alkylation of a cyclohexylidene enolate anion, the aldol reaction, catalytic hydrogenation free radical addition), enantioselective synthesis (chiral

organometal complexes, catalysis by chiral bases, enzyme based processes, enantioselective deprotonation of cyclohexanone derivatives) enantioconvergent synthesis via the Claisen rearrangement.

Group D

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

Chirality in Molecules Devoid of Chiral Centers: Introduction and nomenclature, allenes, synthesis of optically active allenes, determination of configuration, cyclic allenes, alkylidenecyclohexanes, spiranes, biphenyl (atropisomerism), biphenyls 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. Nográdi, *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)

Course No.: CHE-660

Semester: Fourth (4th)

Credit: Four (4) hrs.

Full Marks: 100

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 heteroannular systems, problems.

Infrared Spectroscopy: Introduction, theory, coupling interaction and hydrogen bonding, instrumentation, dispersion IR spectrometer, 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, alcohol, phenol, ether, epoxide, peroxide, ketones, aldehydes, carboxylic acids, ester, acid halides, carboxylic acid, amide, amine etc, problems.

Group B

NMR Spectroscopy (Nuclear Magnetic Resonance Spectroscopy):

¹H-NMR: Introduction, CW NMR spectroscopy, relaxation (longitudinal and transverse), pulse FT¹H-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.

¹³C-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 (¹H¹³C J values), DEPT spectrum, and problems.

Group C

New Dimensions in NMR: Introduction, ¹H-¹H connectivity, Homo J-resolved ¹H-¹H spectroscopy, correlated spectroscopy (COSY), ¹H-¹³C connectivity, J- resolved ¹H¹³C spectroscopy (HET 2DJ), heteronuclear chemical shift correlation (HETCOR), ¹³C-¹³C 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. Harbornet *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

Credit: Six (6) hrs.

Course No.: CHE-662

Full Mark: 150

Semester: Forth (4th)

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.